

For Paul Schulwitz

649

Access DB# 114/69

# SEARCH REQUEST FORM

Scientific and Technical Information Center

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Requester's Full Name: Sabiba Qay Examiner #: 74141 Date: 2/10/04  
Art Unit: 1616 Phone Number 30 20622 Serial Number: 09/867006  
Mail Box and Bldg/Room Location: 4C70 Results-Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.  
\*\*\*\*\*

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: New 7 $\alpha$ , 17 $\alpha$  bis alkylated testosterone

Inventors (please provide full names): Cleve, Arwed et al.

Earliest Priority Filing Date: 12/23/98 PCT/EP99/10355

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Please search for the steroid of for. (1) in cl. 1, where 6 + 7 position + 15 + 16 + 17 position are substituted (optionally). Double bond is always at 4-position i.e 4-ene.

Please see attached sheet (STIC)

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FEB 11 2004

Thank you

## STAFF USE ONLY

Searcher: Schulwitz  
Searcher Phone #: \_\_\_\_\_  
Searcher Location: \_\_\_\_\_  
Date Searcher Picked Up: 2/17  
Date Completed: 2/17  
Searcher Prep & Review Time: 20  
Clerical Prep Time: \_\_\_\_\_  
Online Time: 20

## Type of Search

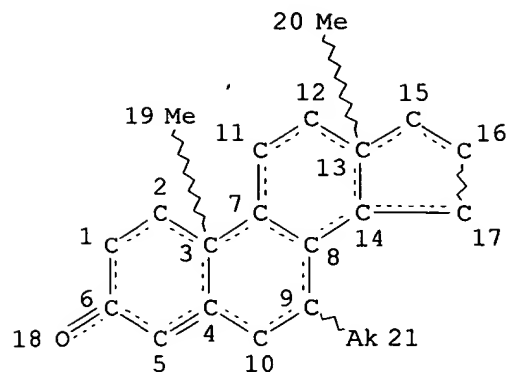
NA Sequence (#) \_\_\_\_\_  
AA Sequence (#) \_\_\_\_\_  
Structure (#) 1  
Bibliographic \_\_\_\_\_  
Litigation \_\_\_\_\_  
Fulltext \_\_\_\_\_  
Patent Family \_\_\_\_\_  
Other \_\_\_\_\_

## Vendors and cost where applicable

STN 300  
Dialog \_\_\_\_\_  
Questel/Orbit \_\_\_\_\_  
Dr. Link \_\_\_\_\_  
Lexis/Nexis \_\_\_\_\_  
Sequence Systems \_\_\_\_\_  
WWW/Internet \_\_\_\_\_  
Other (specify) \_\_\_\_\_

L1

STR



## NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS M6 C AT 21

## GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 21

## STEREO ATTRIBUTES: NONE

L3 154 SEA FILE=REGISTRY SSS FUL L1

L4 9 SEA FILE=HCAPLUS ABB=ON PLU=ON L3

=&gt; d l4 ibib ab hitstr 1-9

L4 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:442168 HCAPLUS

DOCUMENT NUMBER: 133:74180

TITLE: Preparation of new testosterone derivatives and their  
use in the long-term therapy of androgen-dependent  
illnesses

INVENTOR(S): Cleve, Arwed; Sauer, Gerhard; Huwe, Christoph;  
Parczyk, Karsten; Hoffmann, Jens; Schneider, Martin

PATENT ASSIGNEE(S): Schering A.-G., Germany

SOURCE: Ger. Offen., 41 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

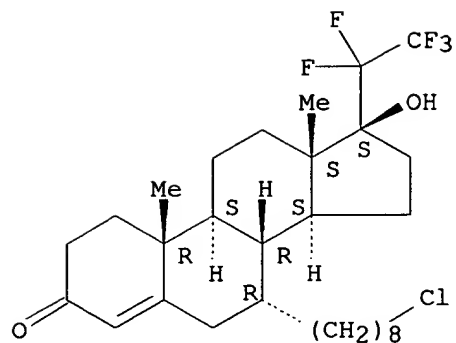
## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19860719	A1	20000629	DE 1998-19860719	19981223
WO 2000039148	A1	20000706	WO 1999-EP10355	19991223

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,  
CZ, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN,  
IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD,  
MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK,

SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ,  
BY, KG, KZ, MD, RU, TJ, TM  
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,  
DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,  
CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
EP 1140972 A1 20011010 EP 1999-967003 19991223  
EP 1140972 B1 20030305  
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IE, SI, LT, LV, FI, RO  
JP 2002533471 T2 20021008 JP 2000-591059 19991223  
AT 233782 E 20030315 AT 1999-967003 19991223  
NO 2001003168 A 20010622 NO 2001-3168 20010622  
PRIORITY APPLN. INFO.: DE 1998-19860719 A 19981223  
WO 1999-EP10355 W 19991223  
OTHER SOURCE(S): MARPAT 133:74180  
AB The available invention concerns new 7.alpha.,17.alpha.,17.beta.-  
substituted testosterone derivs. I [A = C6-13-alkylene; B = O, S(O)p, NY,  
NYCO, NYSO2, OSO2, OSiMe2, SCO, connection between A and CC; p = 0, 1, 2;  
Y = H, C1-8-alkyl, or together with CC a connection between A and CD, CC a  
connection between B and CD, or together with B a connection between A and  
CD, C1-6-alkyl, (un)substituted phenylene, vinyl, C1-4-alkoxy;  
C1-4-alkoxycarbonyl, bis(C1-4-alkoxycarbonyl)methyl] and their use as pure  
anti-androgens in the long-term therapy of androgen-dependent illnesses,  
in particular for the long-term anti-androgen therapy of the prostate  
carcinomas. Thus, antiandrogen II was prepd. from 17.alpha.-methyl-3-  
oxoandrosta-4,6-dien-17.beta.-yl acetate (III). II was tested for  
antiproliferation activity against against human prostate carcinoma LNCaP  
[IC50 = 40 nM].  
IT 278603-67-1P 278603-68-2P 278603-72-8P  
278603-92-2P 278603-97-7P 278604-10-7P  
278604-11-8P 278604-12-9P 278604-20-9P  
278604-21-0P 278604-22-1P 278604-23-2P  
278604-24-3P 278604-25-4P 278604-26-5P  
278604-27-6P 278604-28-7P 278604-30-1P  
278604-31-2P 278604-32-3P 278604-33-4P  
278604-35-6P 278604-36-7P 278604-38-9P  
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278604-42-5P 278604-43-6P 278604-46-9P  
278604-52-7P 278604-57-2P 278604-60-7P  
278604-66-3P 278604-79-8P 278604-80-1P  
278605-00-8P 278605-02-0P 278605-05-3P  
278605-09-7P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT  
(Reactant or reagent); USES (Uses)  
(prepn. of new testosterone derivs. and their use in the long-term  
therapy of androgen-dependent illnesses)  
RN 278603-67-1 HCAPLUS  
CN Pregn-4-en-3-one, 7-(8-chlorooctyl)-20,20,21,21,21-pentafluoro-17-hydroxy-  
, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

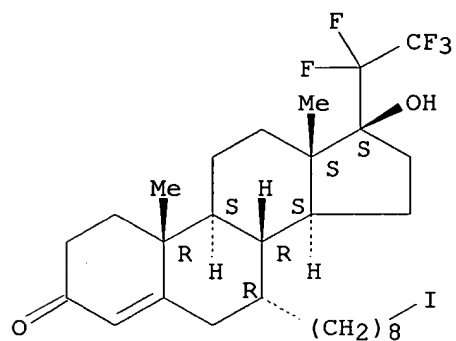
Absolute stereochemistry.



RN 278603-68-2 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-(8-iodooctyl)-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

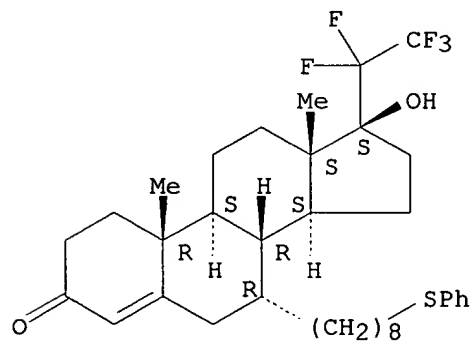
Absolute stereochemistry.



RN 278603-72-8 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[8-(phenylthio)octyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

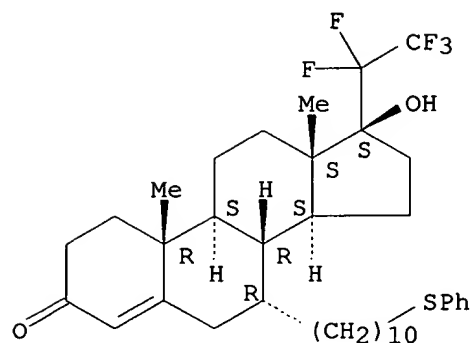
Absolute stereochemistry.



RN 278603-92-2 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[10-(phenylthio)decyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

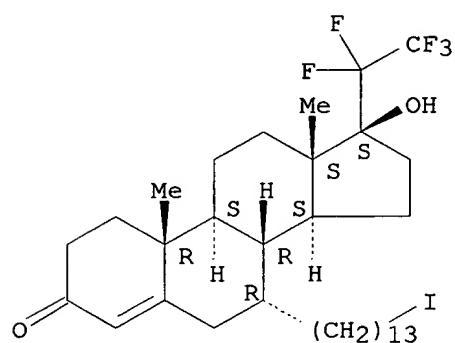
Absolute stereochemistry.



RN 278603-97-7 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-(13-iodotridecyl)-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

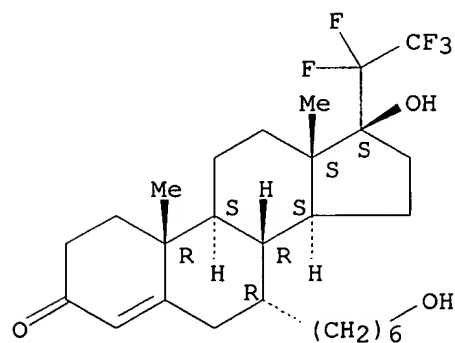
Absolute stereochemistry.



RN 278604-10-7 HCAPLUS

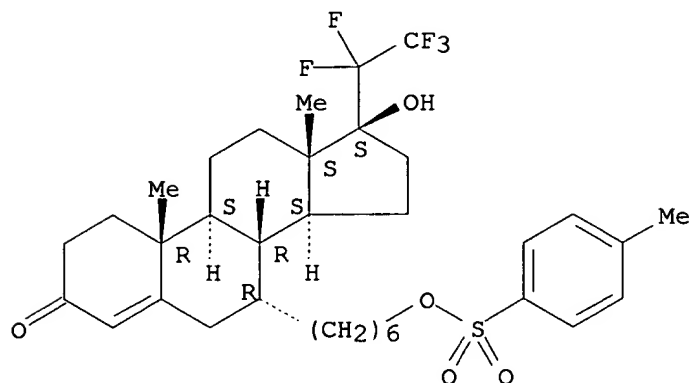
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-(6-hydroxyhexyl)-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



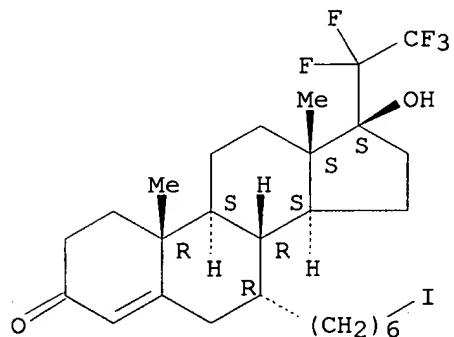
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 CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[6-[[4-methylphenyl)sulfonyl]oxy]hexyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



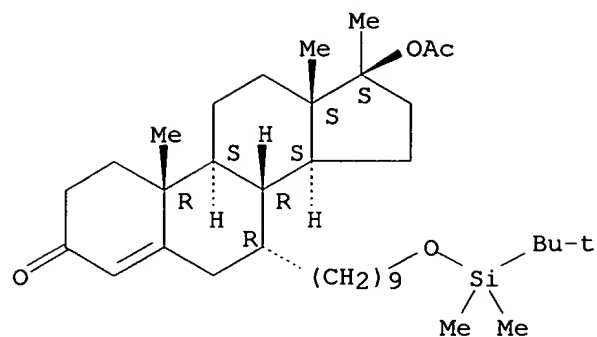
RN 278604-12-9 HCAPLUS  
 CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-(6-iodohexyl)-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 278604-20-9 HCAPLUS  
 CN Androst-4-en-3-one, 17-(acetyloxy)-7-[9-[[[1,1-dimethylethyl)dimethylsilyl]oxy]nonyl]-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

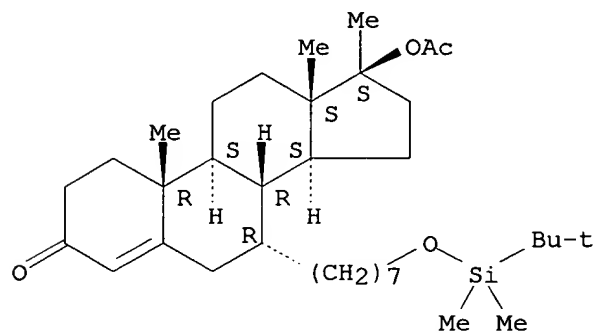
Absolute stereochemistry.



RN 278604-21-0 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-[7-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]heptyl]-17-methyl-, (7.alpha.,17.beta.)-(9CI) (CA INDEX NAME)

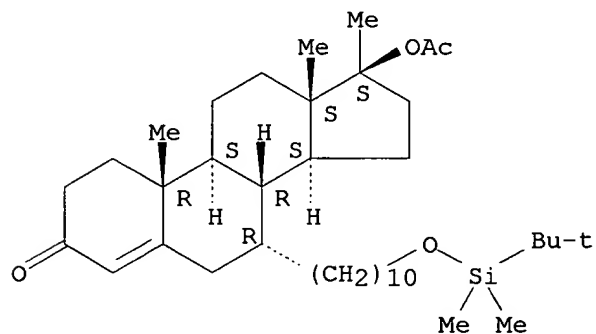
Absolute stereochemistry.



RN 278604-22-1 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-[10-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]decyl]-17-methyl-, (7.alpha.,17.beta.)-(9CI) (CA INDEX NAME)

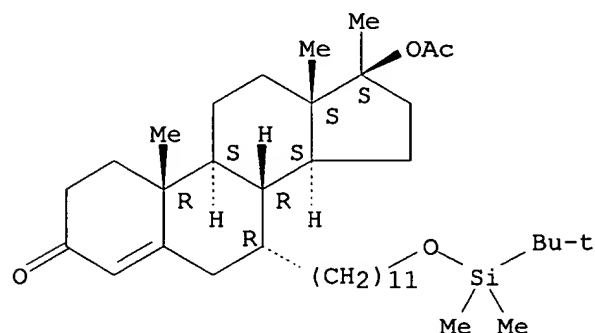
Absolute stereochemistry.



RN 278604-23-2 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-[11-[[{1,1-dimethylethyl}dimethylsilyl]oxy]undecyl]-17-methyl-, (7.alpha.,17.beta.)-(9CI) (CA INDEX NAME)

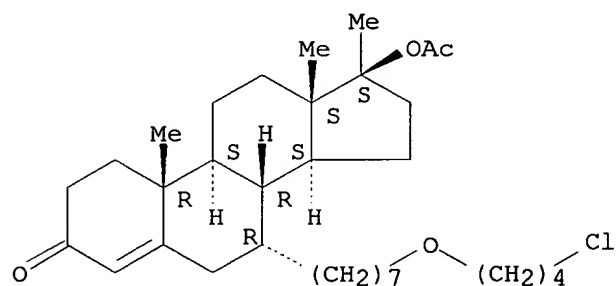
Absolute stereochemistry.



RN 278604-24-3 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-[7-(4-chlorobutoxy)heptyl]-17-methyl-, (7.alpha.,17.beta.)-(9CI) (CA INDEX NAME)

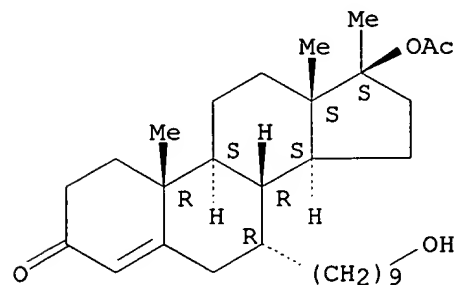
Absolute stereochemistry.



RN 278604-25-4 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-(9-hydroxynonyl)-17-methyl-, (7.alpha.,17.beta.)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

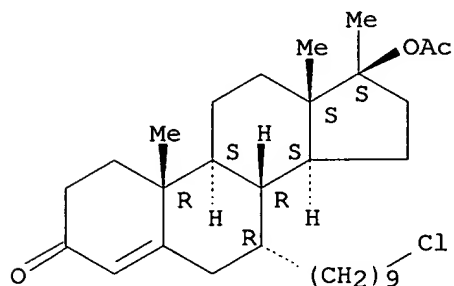


RN 278604-26-5 HCAPLUS



CN Androst-4-en-3-one, 17-(acetyloxy)-7-(9-chlorononyl)-17-methyl-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

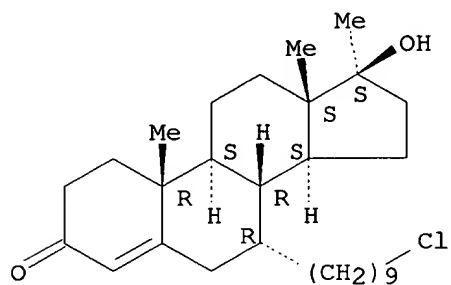
Absolute stereochemistry.



RN 278604-27-6 HCAPLUS

CN Androst-4-en-3-one, 7-(9-chlorononyl)-17-hydroxy-17-methyl-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

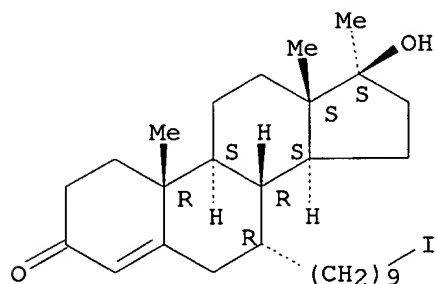
Absolute stereochemistry.



RN 278604-28-7 HCAPLUS

CN Androst-4-en-3-one, 17-hydroxy-7-(9-iodononyl)-17-methyl-,  
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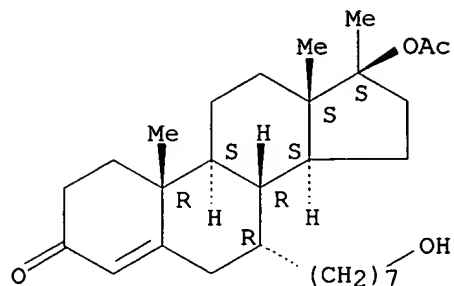
Absolute stereochemistry.



RN 278604-30-1 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-(7-hydroxyheptyl)-17-methyl-,  
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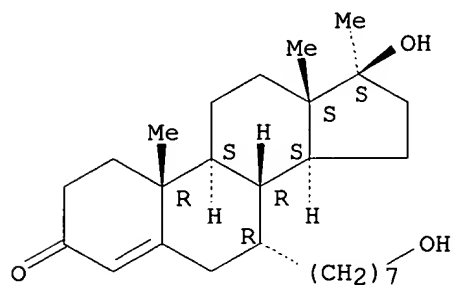
Absolute stereochemistry.



RN 278604-31-2 HCAPLUS

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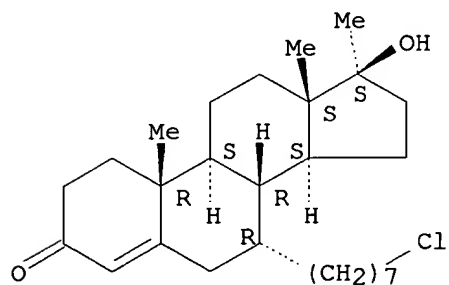
Absolute stereochemistry.



RN 278604-32-3 HCAPLUS

CN Androst-4-en-3-one, 7-(7-chloroheptyl)-17-hydroxy-17-methyl-,  
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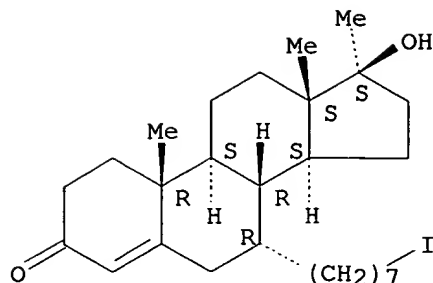
Absolute stereochemistry.



RN 278604-33-4 HCAPLUS

CN Androst-4-en-3-one, 17-hydroxy-7-(7-iodoheptyl)-17-methyl-,  
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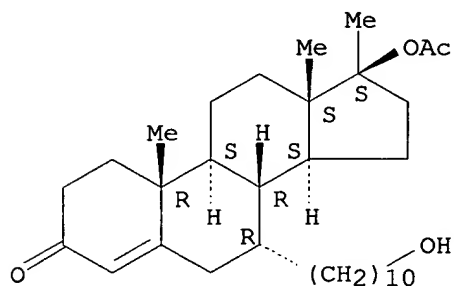
Absolute stereochemistry.



RN 278604-35-6 HCAPLUS

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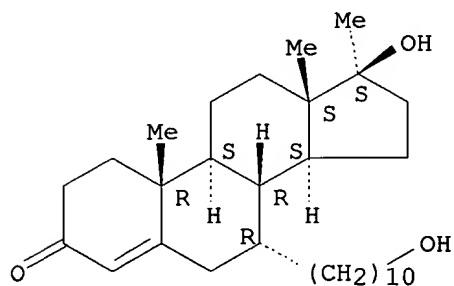
Absolute stereochemistry.



RN 278604-36-7 HCAPLUS

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(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

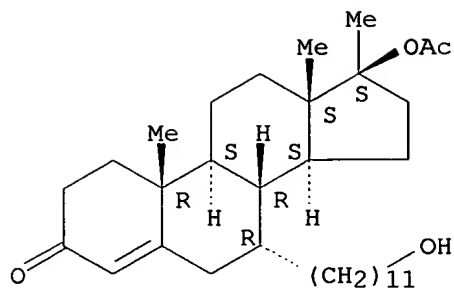
Absolute stereochemistry.



RN 278604-38-9 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-(11-hydroxyundecyl)-17-methyl-,  
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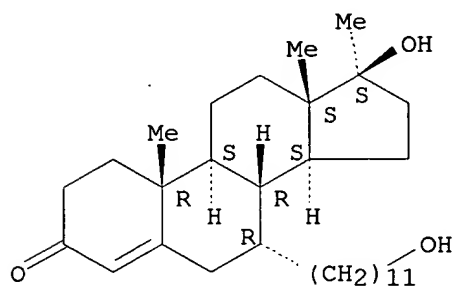
Absolute stereochemistry.



RN 278604-39-0 HCAPLUS

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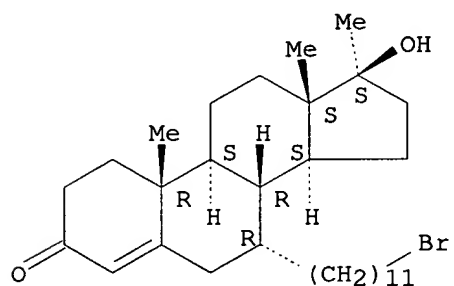
Absolute stereochemistry.



RN 278604-40-3 HCAPLUS

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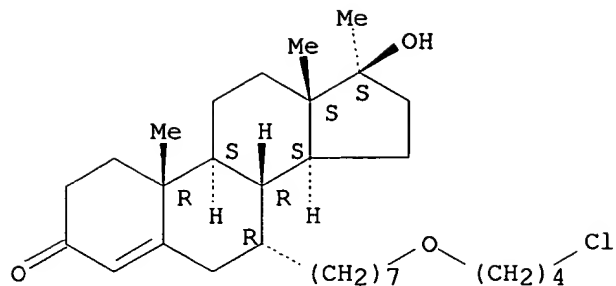
Absolute stereochemistry.



RN 278604-41-4 HCAPLUS

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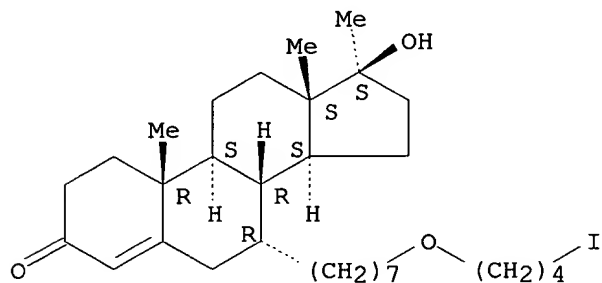
Absolute stereochemistry.



RN 278604-42-5 HCAPLUS

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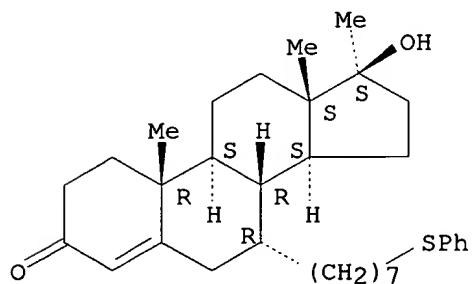
Absolute stereochemistry.



RN 278604-43-6 HCAPLUS

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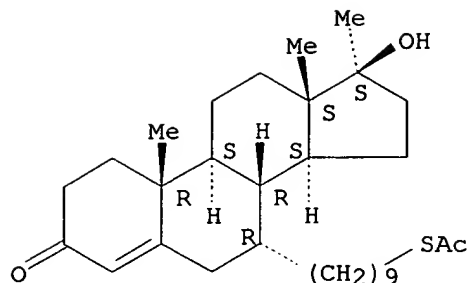
Absolute stereochemistry.



RN 278604-46-9 HCAPLUS

CN Androst-4-en-3-one, 7-[9-(acetylthio)nonyl]-17-hydroxy-17-methyl-,  
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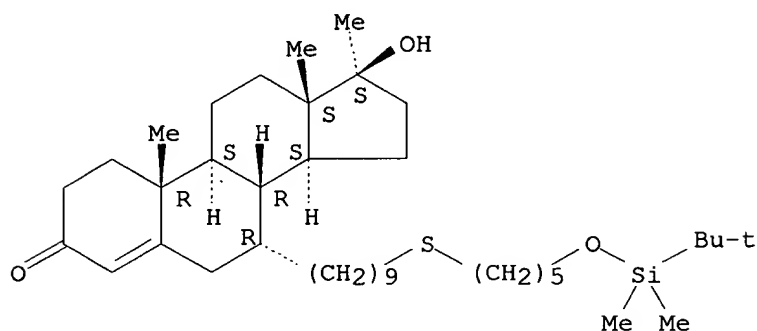
Absolute stereochemistry.



RN 278604-52-7 HCAPLUS

CN Androst-4-en-3-one, 7-[9-[[5-[[[1,1-dimethylethyl]dimethylsilyl]oxy]pentyl]thio]nonyl]-17-hydroxy-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

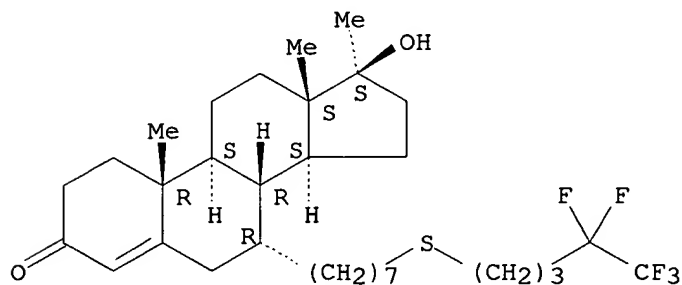
Absolute stereochemistry.



RN 278604-57-2 HCAPLUS

CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[7-[(4,4,5,5,5-pentafluoropentyl)thio]heptyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

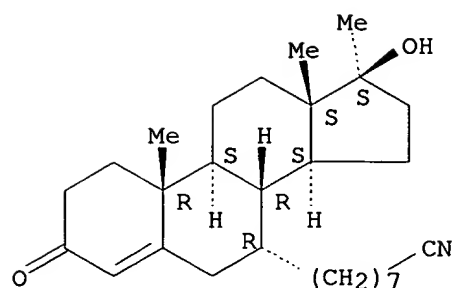
Absolute stereochemistry.



RN 278604-60-7 HCAPLUS

CN Androst-4-ene-7-octanenitrile, 17-hydroxy-17-methyl-3-oxo-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

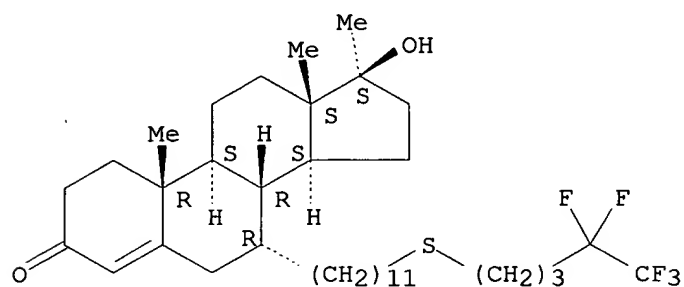
Absolute stereochemistry.



RN 278604-66-3 HCAPLUS

CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[(4,4,5,5,5-pentafluoropentyl)thio]undecyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

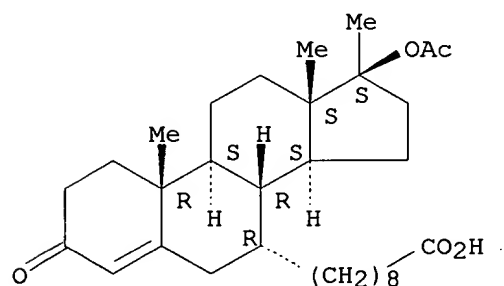
Absolute stereochemistry.



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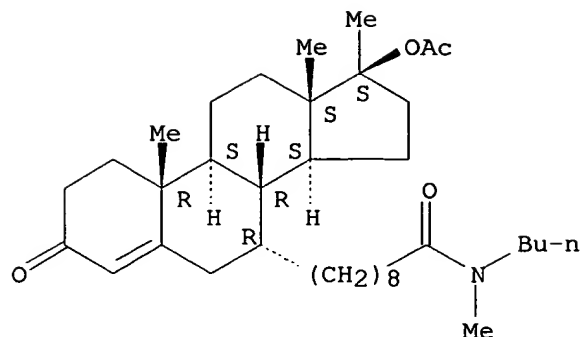
Absolute stereochemistry.



RN 278604-80-1 HCAPLUS

CN Androst-4-ene-7-nonanamide, 17-(acetyloxy)-N-butyl-N,17-dimethyl-3-oxo-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

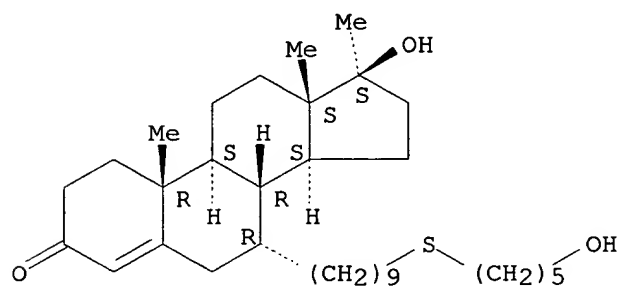
Absolute stereochemistry.



RN 278605-00-8 HCAPLUS

CN Androst-4-en-3-one, 17-hydroxy-7-[9-[(5-hydroxypentyl)thio]nonyl]-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

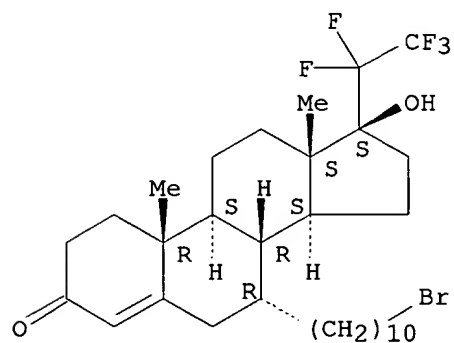
Absolute stereochemistry.



RN 278605-02-0 HCAPLUS

CN Pregn-4-en-3-one, 7-(10-bromodecyl)-20,20,21,21,21-pentafluoro-17-hydroxy-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

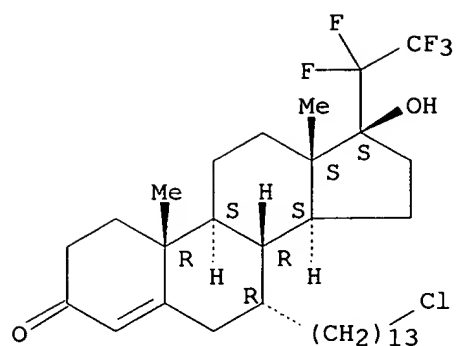


RN 278605-05-3 HCAPLUS

CN Pregn-4-en-3-one, 7-(13-chlorotridecyl)-20,20,21,21,21-pentafluoro-17-hydroxy-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

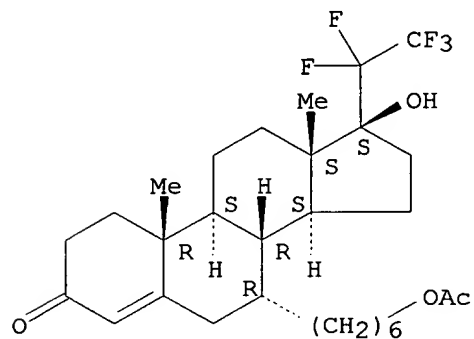




RN 278605-09-7 HCAPLUS

CN Pregn-4-en-3-one, 7-[6-(acetyloxy)hexyl]-20,20,21,21,21-pentafluoro-17-hydroxy-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 278603-70-6P 278603-74-0P 278603-75-1P  
 278603-76-2P 278603-77-3P 278603-79-5P  
 278603-81-9P 278603-82-0P 278603-83-1P  
 278603-84-2P 278603-85-3P 278603-86-4P  
 278603-88-6P 278603-89-7P 278603-94-4P  
 278603-98-8P 278604-00-5P 278604-01-6P  
 278604-02-7P 278604-03-8P 278604-04-9P  
 278604-05-0P 278604-06-1P 278604-07-2P  
 278604-08-3P 278604-13-0P 278604-14-1P  
 278604-15-2P 278604-16-3P 278604-17-4P  
 278604-18-5P 278604-19-6P 278604-29-8P  
 278604-34-5P 278604-37-8P 278604-44-7P  
 278604-45-8P 278604-47-0P 278604-48-1P  
 278604-49-2P 278604-50-5P 278604-51-6P  
 278604-53-8P 278604-54-9P 278604-55-0P  
 278604-56-1P 278604-58-3P 278604-59-4P  
 278604-61-8P 278604-62-9P 278604-63-0P  
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 278604-71-0P 278604-72-1P 278604-73-2P  
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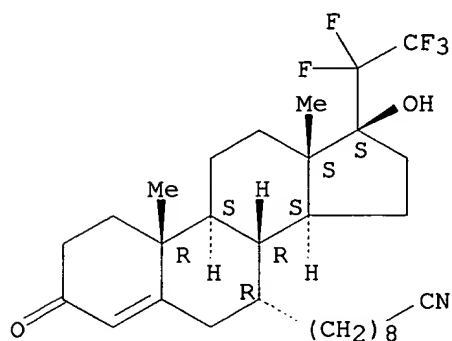
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 278604-85-6P 278604-86-7P 278604-87-8P  
 278604-88-9P 278604-89-0P 278604-90-3P  
 278604-91-4P 278604-92-5P 278604-93-6P  
 278604-94-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of new testosterone derivs. and their use in the long-term therapy of androgen-dependent illnesses)

RN 278603-70-6 HCAPLUS

CN Pregn-4-ene-7-nonanenitrile, 20,20,21,21,21-pentafluoro-17-hydroxy-3-oxo-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

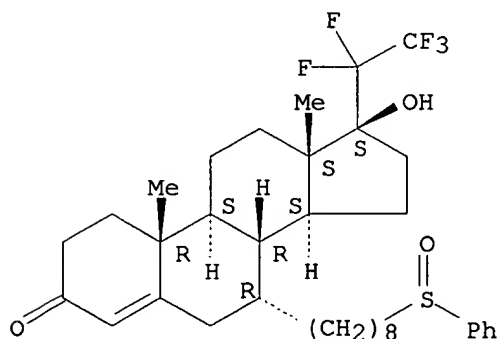
Absolute stereochemistry.



RN 278603-74-0 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[8-(phenylsulfinyl)octyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

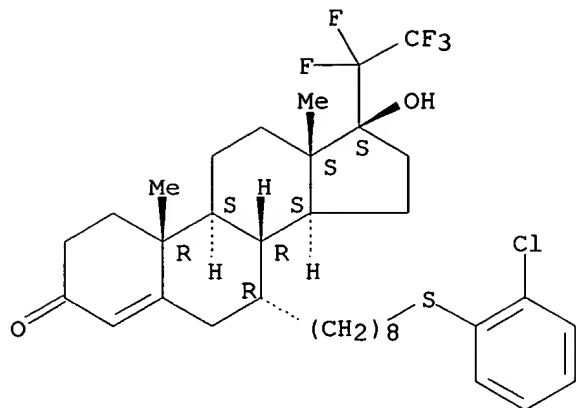
Absolute stereochemistry.



RN 278603-75-1 HCAPLUS

CN Pregn-4-en-3-one, 7-[8-[(2-chlorophenyl)thio]octyl]-20,20,21,21,21-pentafluoro-17-hydroxy-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

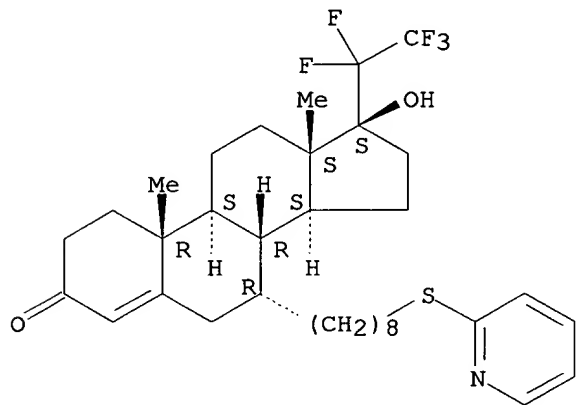
Absolute stereochemistry.



RN 278603-76-2 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[8-(2-pyridinylthio)octyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

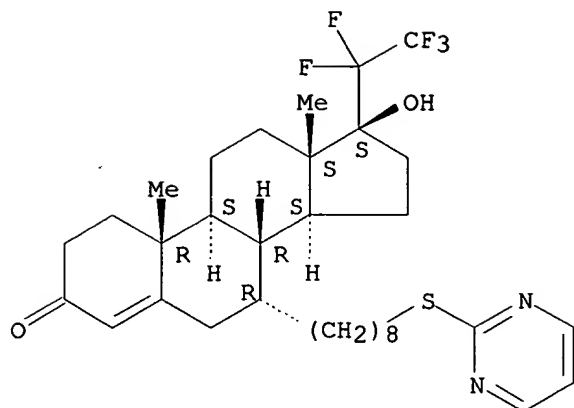
Absolute stereochemistry.



RN 278603-77-3 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[8-(2-pyrimidinylthio)octyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

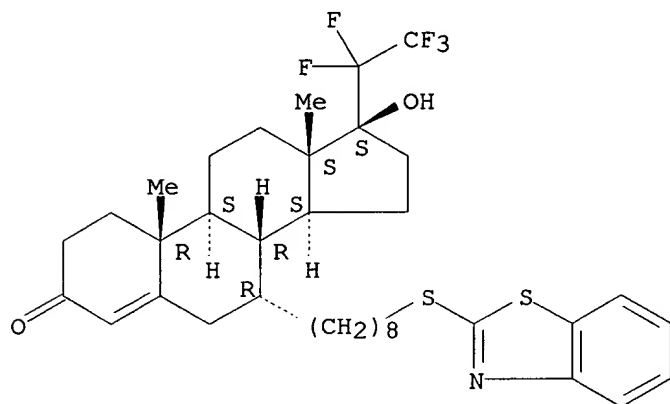
Absolute stereochemistry.



RN 278603-79-5 HCAPLUS

CN Pregn-4-en-3-one, 7-[8-(2-benzothiazolylthio)octyl]-20,20,21,21,21-pentafluoro-17-hydroxy-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

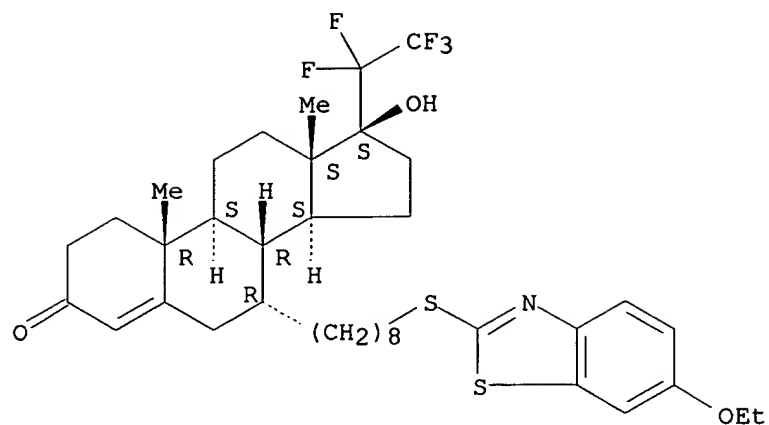
Absolute stereochemistry.



RN 278603-81-9 HCAPLUS

CN Pregn-4-en-3-one, 7-[8-[(6-ethoxy-2-benzothiazolyl)thio]octyl]-20,20,21,21,21-pentafluoro-17-hydroxy-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

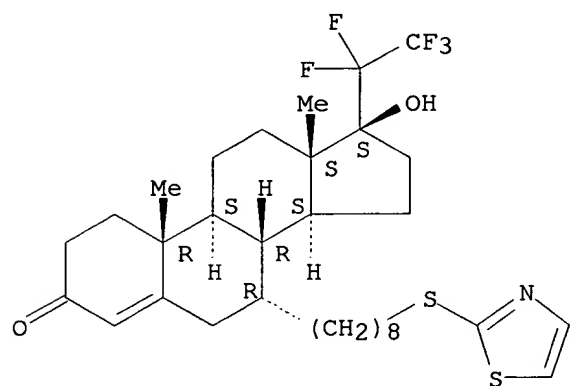
Absolute stereochemistry.



RN 278603-82-0 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[8-(2-thiazolylthio)octyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

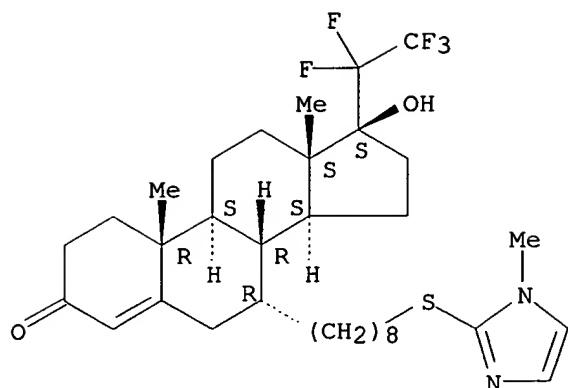
Absolute stereochemistry.



RN 278603-83-1 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[8-[(1-methyl-1H-imidazol-2-yl)thio]octyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

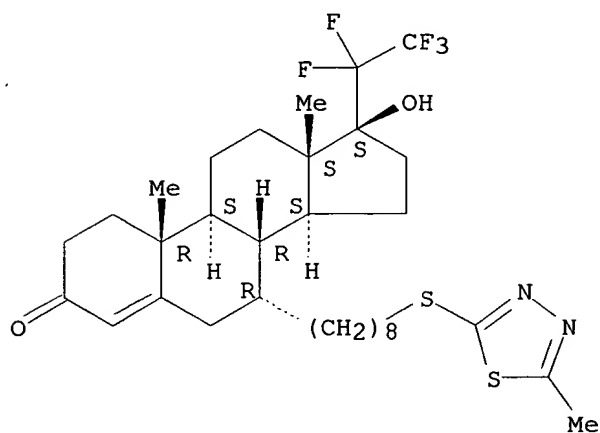
Absolute stereochemistry.



RN 278603-84-2 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[8-[(5-methyl-1,3,4-thiadiazol-2-yl)thio]octyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

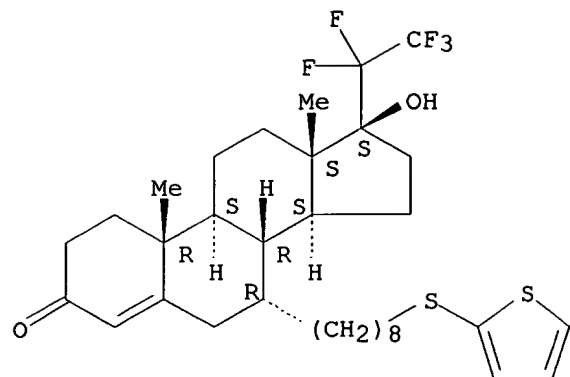
Absolute stereochemistry.



RN 278603-85-3 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[8-(2-thienylthio)octyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

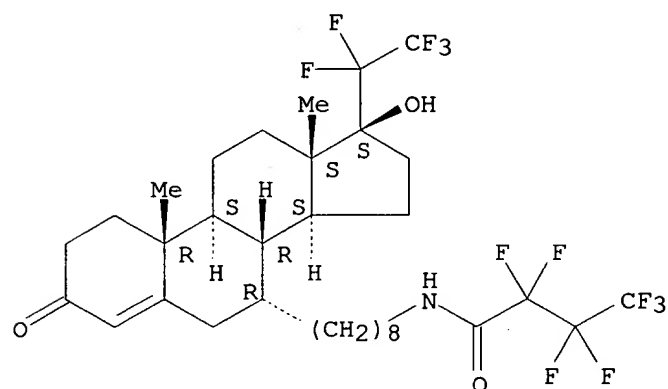
Absolute stereochemistry.



RN 278603-86-4 HCAPLUS

CN Butanamide, 2,2,3,3,4,4,4-heptafluoro-N-[8-[(7.alpha.,17.alpha.)-20,20,21,21,21-pentafluoro-17-hydroxy-3-oxopregn-4-en-7-yl]octyl]- (9CI)  
(CA INDEX NAME)

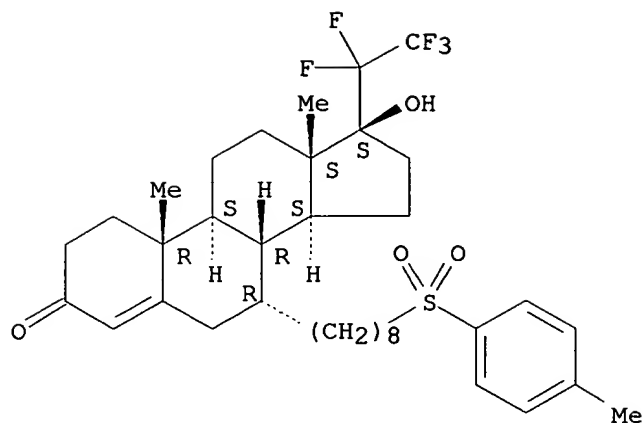
Absolute stereochemistry.



RN 278603-88-6 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[8-[(4-methylphenyl)sulfonyl]octyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

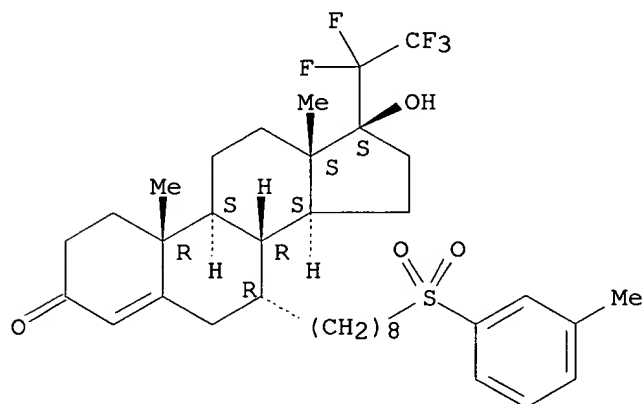
Absolute stereochemistry.



RN 278603-89-7 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[8-[(3-methylphenyl)sulfonyl]octyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

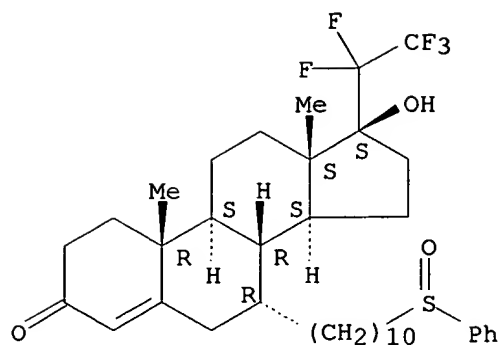


RN 278603-94-4 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[10-(phenylsulfinyl)decyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

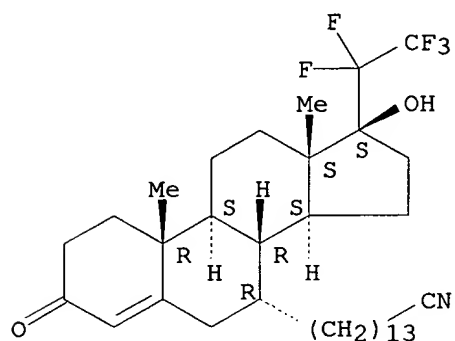




RN 278603-98-8 HCAPLUS

CN Pregn-4-ene-7-tetradecanenitrile, 20,20,21,21,21-pentafluoro-17-hydroxy-3-oxo-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

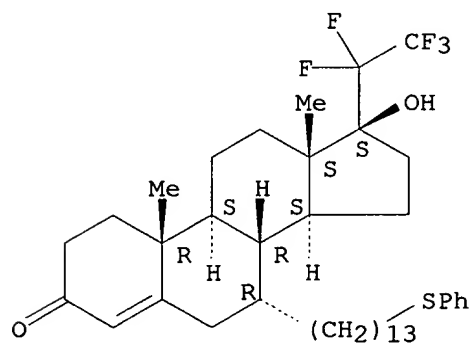
Absolute stereochemistry.



RN 278604-00-5 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[13-(phenylthio)tridecyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

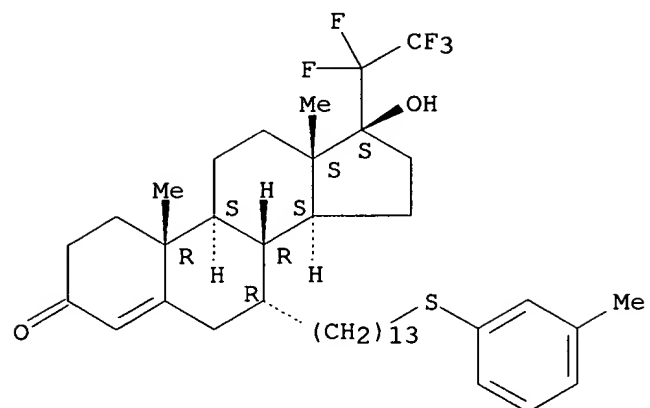
Absolute stereochemistry.



RN 278604-01-6 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[13-[(3-methylphenyl)thio]tridecyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

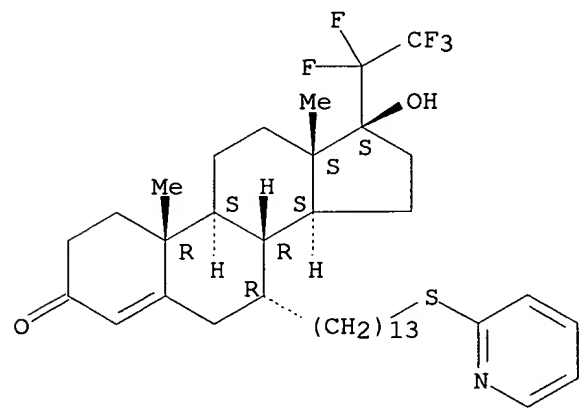
Absolute stereochemistry.



RN 278604-02-7 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[13-(2-pyridinylthio)tridecyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

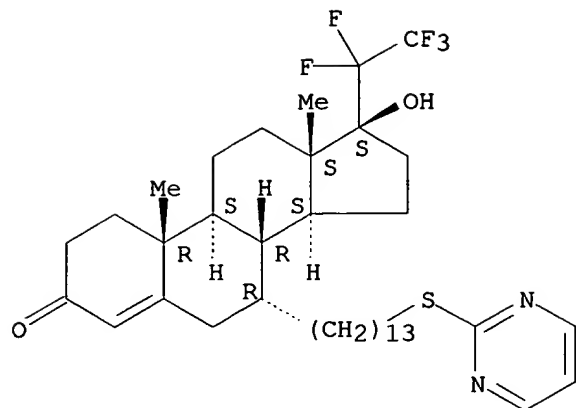
Absolute stereochemistry.



RN 278604-03-8 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[13-(2-pyrimidinylthio)tridecyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

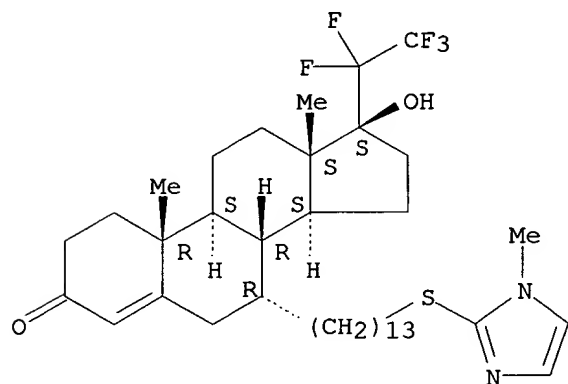
Absolute stereochemistry.



RN 278604-04-9 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[13-[(1-methyl-1H-imidazol-2-yl)thio]tridecyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

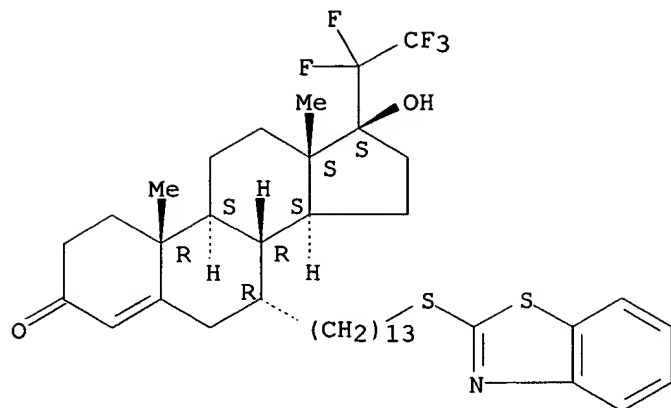
Absolute stereochemistry.



RN 278604-05-0 HCAPLUS

CN Pregn-4-en-3-one, 7-[13-(2-methyl-1H-imidazol-5-yl)thio]tridecyl]-20,20,21,21,21-pentafluoro-17-hydroxy-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

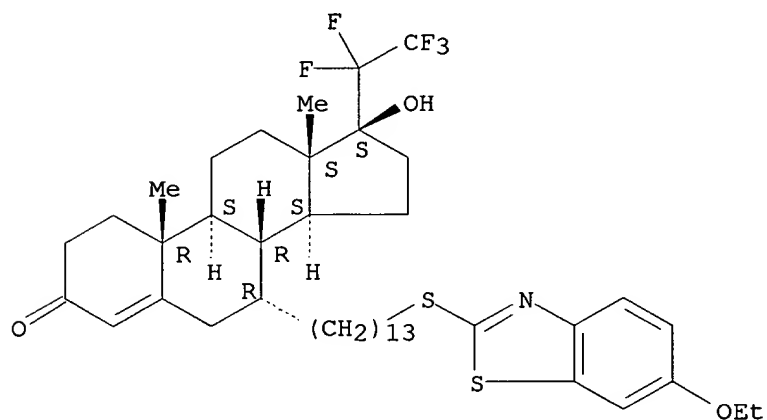
Absolute stereochemistry.



RN 278604-06-1 HCAPLUS

CN Pregn-4-en-3-one, 7-[13-[(6-ethoxy-2-benzothiazolyl)thio]tridecyl]-  
20,20,21,21,21-pentafluoro-17-hydroxy-, (7.alpha.,17.alpha.)- (9CI) (CA  
INDEX NAME)

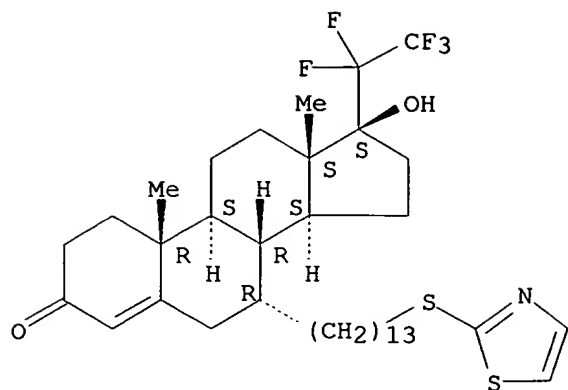
Absolute stereochemistry.



RN 278604-07-2 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[13-(2-  
thiazolylthio)tridecyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

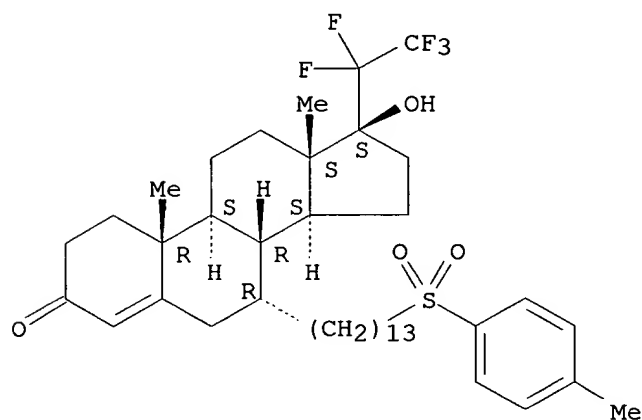
Absolute stereochemistry.



RN 278604-08-3 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[13-[(4-methylphenyl)sulfonyl]tridecyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

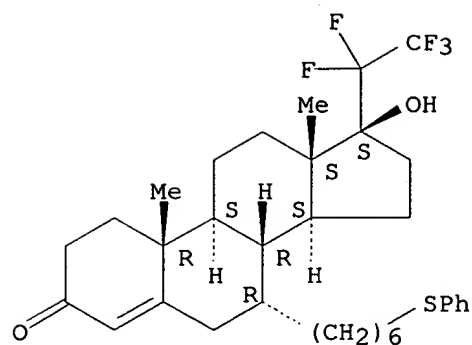
Absolute stereochemistry.



RN 278604-13-0 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[6-(phenylthio)hexyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

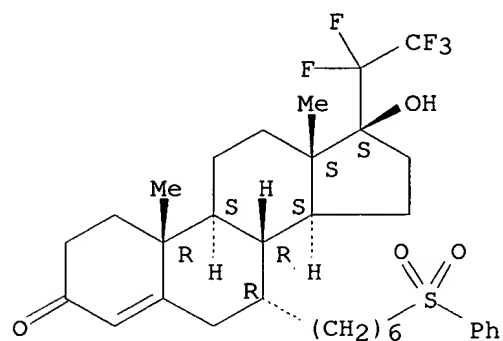
Absolute stereochemistry.



RN 278604-14-1 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[6-(phenylsulfonyl)hexyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

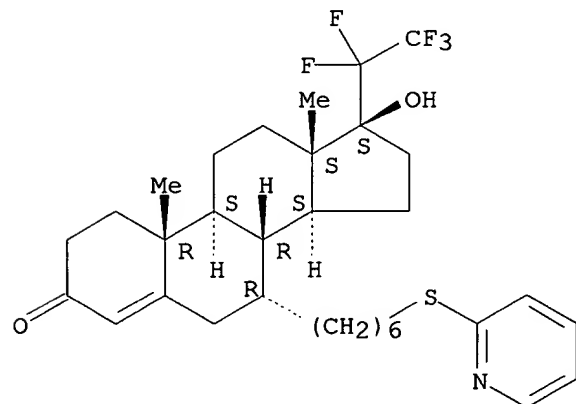
Absolute stereochemistry.



RN 278604-15-2 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[6-(2-pyridinylthio)hexyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

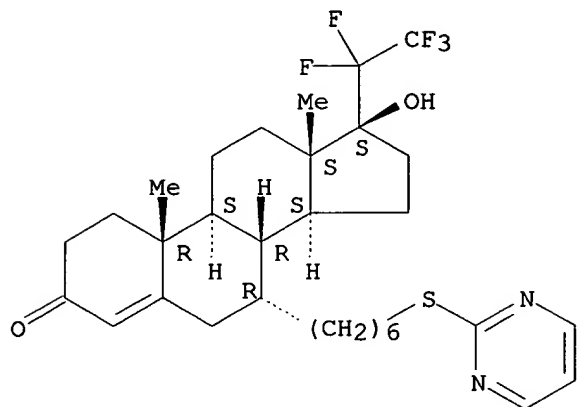
Absolute stereochemistry.



RN 278604-16-3 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[6-(2-pyrimidinylthio)hexyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

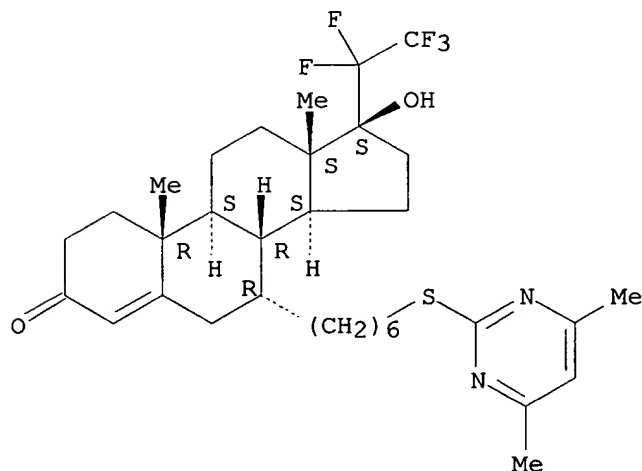
Absolute stereochemistry.



RN 278604-17-4 HCAPLUS

CN Pregn-4-en-3-one, 7-[6-[(4,6-dimethyl-2-pyrimidinyl)thio]hexyl]-20,20,21,21,21-pentafluoro-17-hydroxy-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

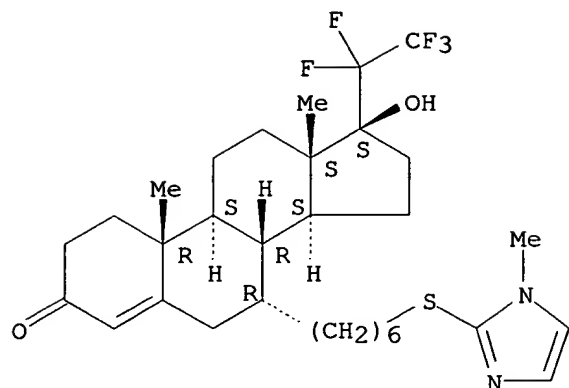
Absolute stereochemistry.



RN 278604-18-5 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[6-[(1-methyl-1H-imidazol-2-yl)thio]hexyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

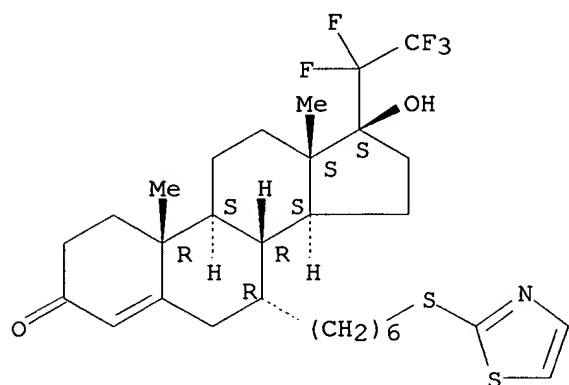
Absolute stereochemistry.



RN 278604-19-6 HCAPLUS

CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[6-(2-thiazolylthio)hexyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

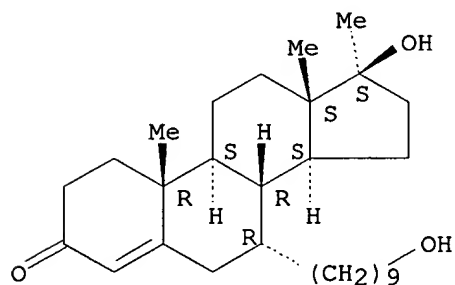
Absolute stereochemistry.



RN 278604-29-8 HCAPLUS

CN Androst-4-en-3-one, 17-hydroxy-7-(9-hydroxynonyl)-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

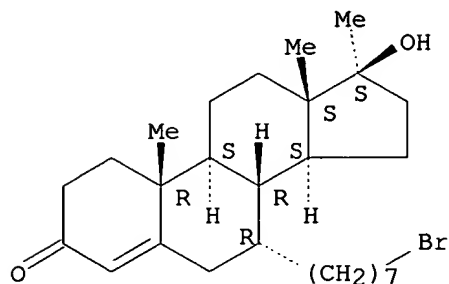


RN 278604-34-5 HCAPLUS



CN Androst-4-en-3-one, 7-(7-bromoheptyl)-17-hydroxy-17-methyl-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

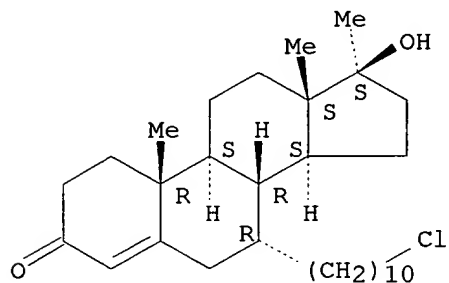
Absolute stereochemistry.



RN 278604-37-8 HCAPLUS

CN Androst-4-en-3-one, 7-(10-chlorodecyl)-17-hydroxy-17-methyl-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

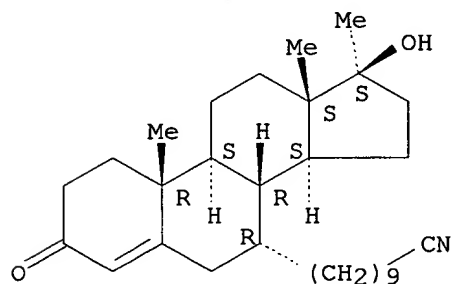
Absolute stereochemistry.



RN 278604-44-7 HCAPLUS

CN Androst-4-ene-7-decanenitrile, 17-hydroxy-17-methyl-3-oxo-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

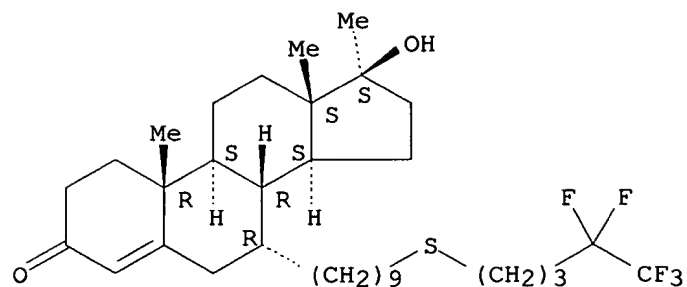
Absolute stereochemistry.



RN 278604-45-8 HCAPLUS

CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[9-[(4,4,5,5,5-pentafluoropentyl)thio]nonyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

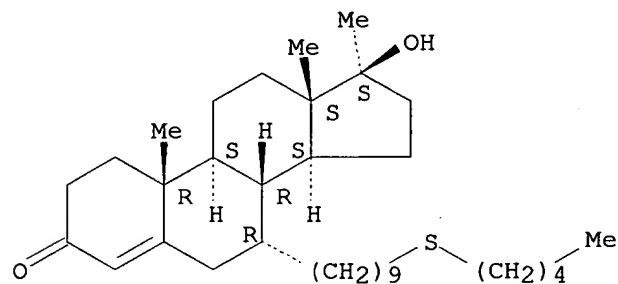
Absolute stereochemistry.



RN 278604-47-0 HCAPLUS

CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[9-(pentylthio)nonyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

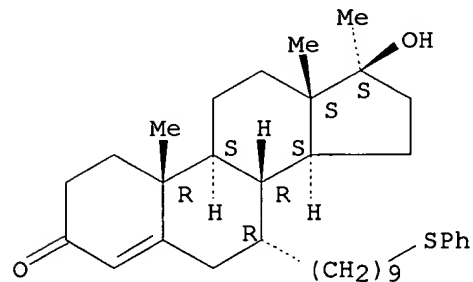
Absolute stereochemistry.



RN 278604-48-1 HCAPLUS

CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[9-(phenylthio)nonyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

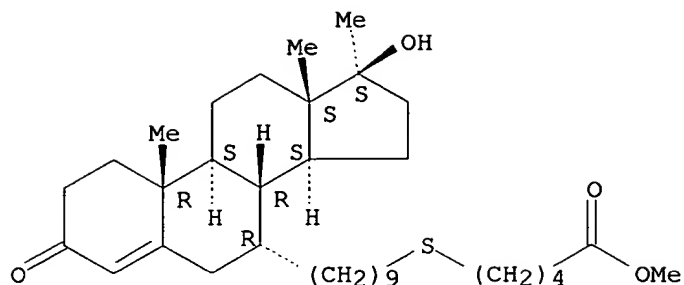
Absolute stereochemistry.



RN 278604-49-2 HCAPLUS

CN Pentanoic acid, 5-[[9-[(7.alpha.,17.beta.)-17-hydroxy-17-methyl-3-oxoandrost-4-en-7-yl]nonyl]thio]-, methyl ester (9CI) (CA INDEX NAME)

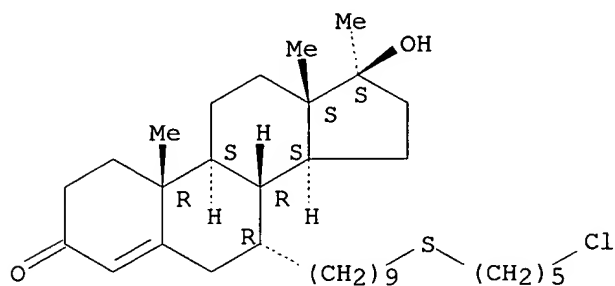
Absolute stereochemistry.



RN 278604-50-5 HCAPLUS

CN Androst-4-en-3-one, 7-[9-[(5-chloropentyl)thio]nonyl]-17-hydroxy-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

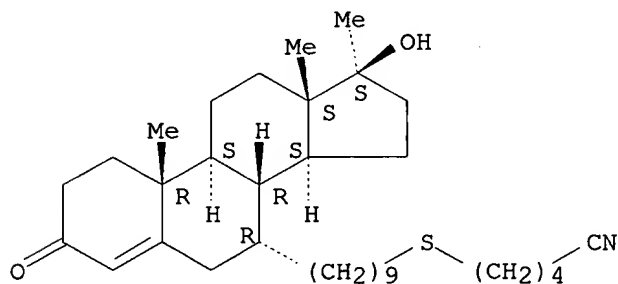
Absolute stereochemistry.



RN 278604-51-6 HCAPLUS

CN Pentanenitrile, 5-[[9-[(7.alpha.,17.beta.)-17-hydroxy-17-methyl-3-oxoandrost-4-en-7-yl]nonyl]thio]- (9CI) (CA INDEX NAME)

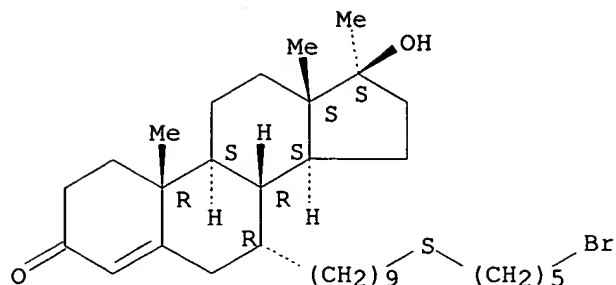
Absolute stereochemistry.



RN 278604-53-8 HCAPLUS

CN Androst-4-en-3-one, 7-[9-[(5-bromopentyl)thio]nonyl]-17-hydroxy-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

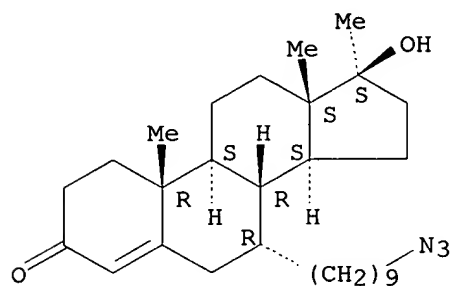
Absolute stereochemistry.



RN 278604-54-9 HCAPLUS

CN Androst-4-en-3-one, 7-(9-azidononyl)-17-hydroxy-17-methyl-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

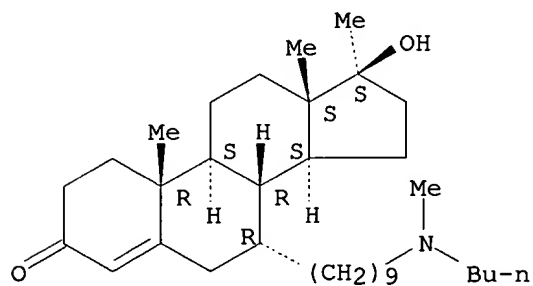
Absolute stereochemistry.



RN 278604-55-0 HCAPLUS

CN Androst-4-en-3-one, 7-[9-(butylmethylamino)nonyl]-17-hydroxy-17-methyl-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

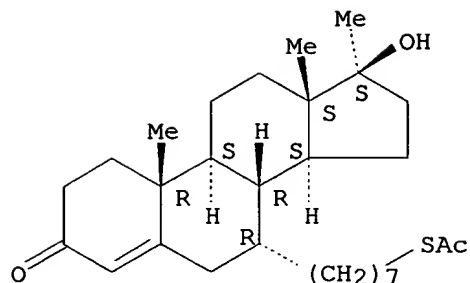
Absolute stereochemistry.



RN 278604-56-1 HCAPLUS

CN Androst-4-en-3-one, 7-[7-(acetylthio)heptyl]-17-hydroxy-17-methyl-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

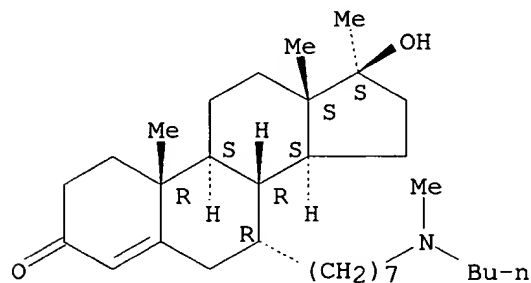
Absolute stereochemistry.



RN 278604-58-3 HCAPLUS

CN Androst-4-en-3-one, 7-[7-(butylmethylamino)heptyl]-17-hydroxy-17-methyl-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

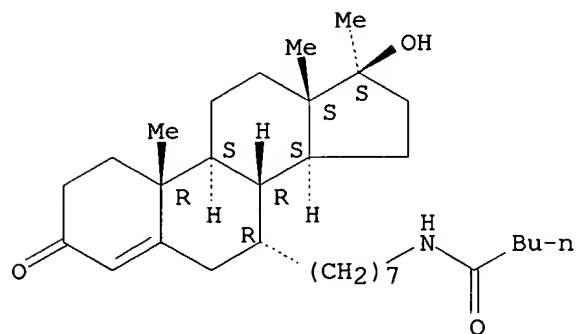
Absolute stereochemistry.



RN 278604-59-4 HCAPLUS

CN Pentanamide, N-[7-[(7.alpha.,17.beta.)-17-hydroxy-17-methyl-3-oxoandrost-4-en-7-yl]heptyl]- (9CI) (CA INDEX NAME)

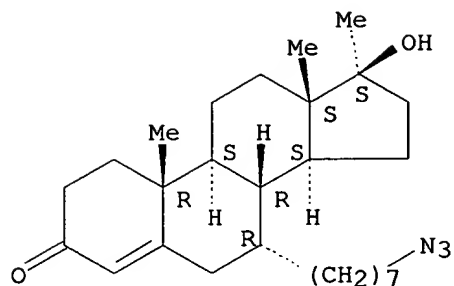
Absolute stereochemistry.



RN 278604-61-8 HCAPLUS

CN Androst-4-en-3-one, 7-(7-azidoheptyl)-17-hydroxy-17-methyl-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

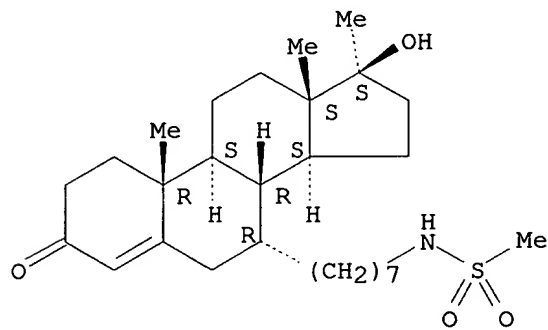
Absolute stereochemistry.



RN 278604-62-9 HCAPLUS

CN Methanesulfonamide, N-[7-[(7.alpha.,17.beta.)-17-hydroxy-17-methyl-3-oxoandrost-4-en-7-yl]heptyl]- (9CI) (CA INDEX NAME)

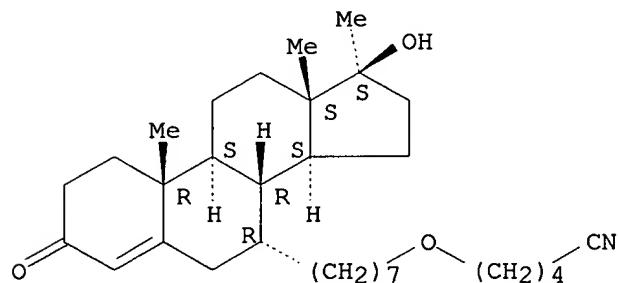
Absolute stereochemistry.



RN 278604-63-0 HCAPLUS

CN Pentanenitrile, 5-[[7-[(7.alpha.,17.beta.)-17-hydroxy-17-methyl-3-oxoandrost-4-en-7-yl]heptyl]oxy]- (9CI) (CA INDEX NAME)

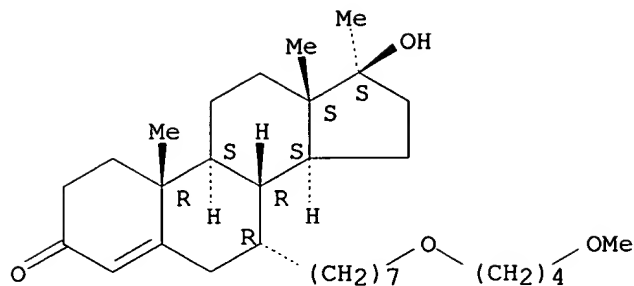
Absolute stereochemistry.



RN 278604-64-1 HCAPLUS

CN Androst-4-en-3-one, 17-hydroxy-7-[7-(4-methoxybutoxy)heptyl]-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

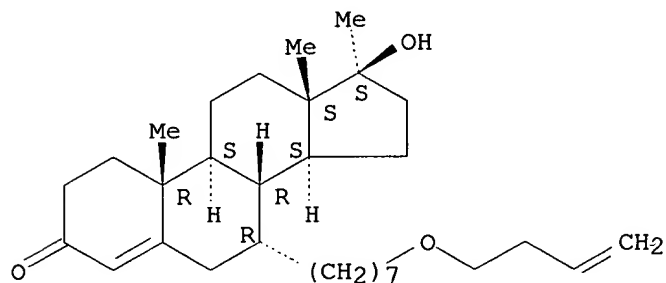
Absolute stereochemistry.



RN 278604-65-2 HCAPLUS

CN Androst-4-en-3-one, 7-[7-(3-butenyloxy)heptyl]-17-hydroxy-17-methyl-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

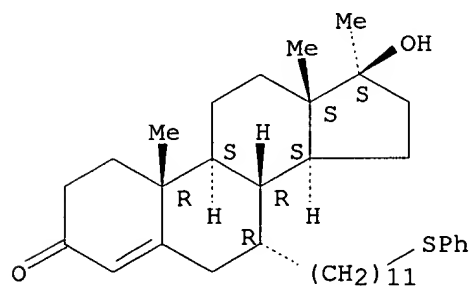
Absolute stereochemistry.



RN 278604-67-4 HCAPLUS

CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[11-(phenylthio)undecyl]-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

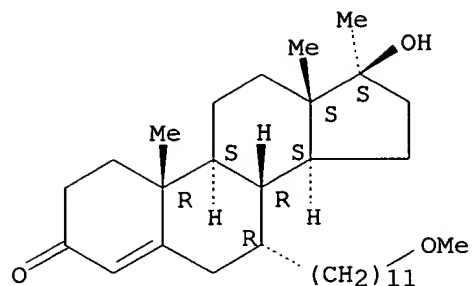
Absolute stereochemistry.



RN 278604-68-5 HCAPLUS

CN Androst-4-en-3-one, 17-hydroxy-7-(11-methoxyundecyl)-17-methyl-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

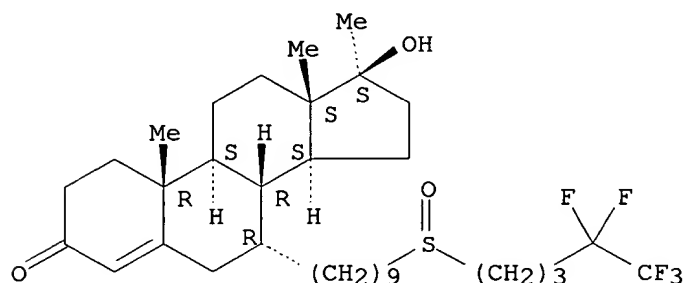
Absolute stereochemistry.



RN 278604-69-6 HCAPLUS

CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

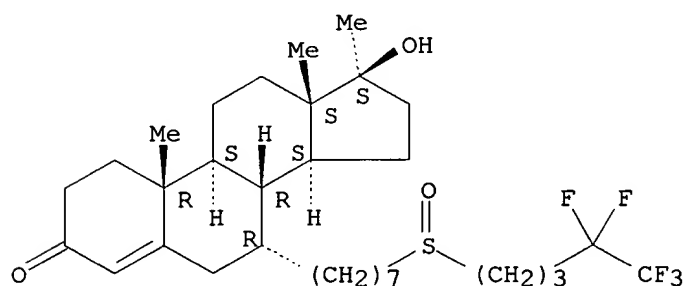
Absolute stereochemistry.



RN 278604-70-9 HCAPLUS

CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[7-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]heptyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

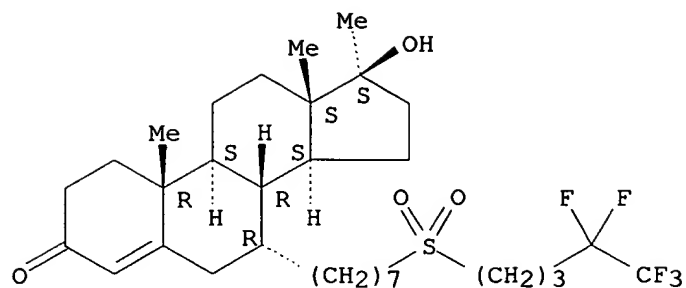


RN 278604-71-0 HCAPLUS

CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[7-[(4,4,5,5,5-pentafluoropentyl)sulfonyl]heptyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

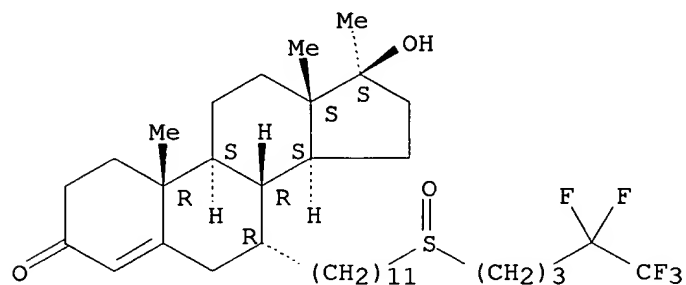




RN 278604-72-1 HCAPLUS

CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[11-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]undecyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

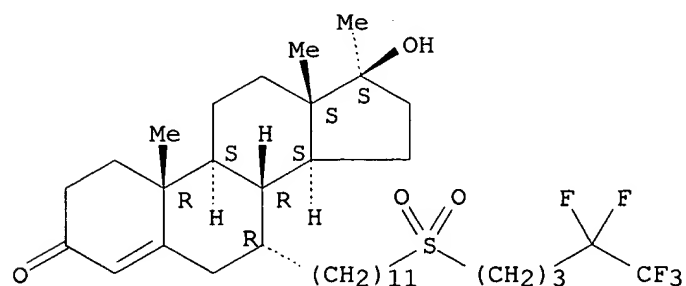
Absolute stereochemistry.



RN 278604-73-2 HCAPLUS

CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[11-[(4,4,5,5,5-pentafluoropentyl)sulfonyl]undecyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

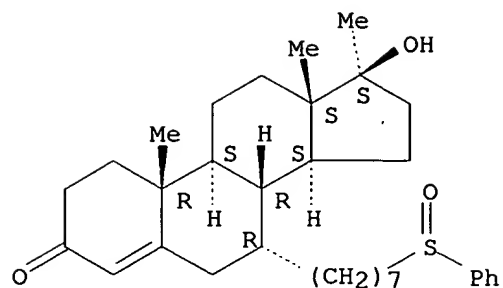
Absolute stereochemistry.



RN 278604-74-3 HCAPLUS

CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[7-(phenylsulfinyl)heptyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

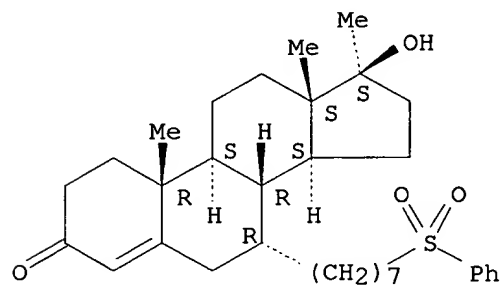
Absolute stereochemistry.



RN 278604-75-4 HCAPLUS

CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[7-(phenylsulfonyl)heptyl]-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

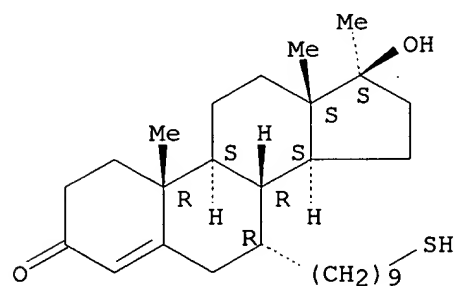
Absolute stereochemistry.



RN 278604-76-5 HCAPLUS

CN Androst-4-en-3-one, 17-hydroxy-7-(9-mercaptononyl)-17-methyl-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

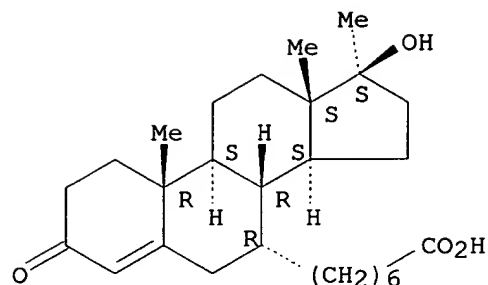
Absolute stereochemistry.



RN 278604-77-6 HCAPLUS

CN Androst-4-ene-7-heptanoic acid, 17-hydroxy-17-methyl-3-oxo-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

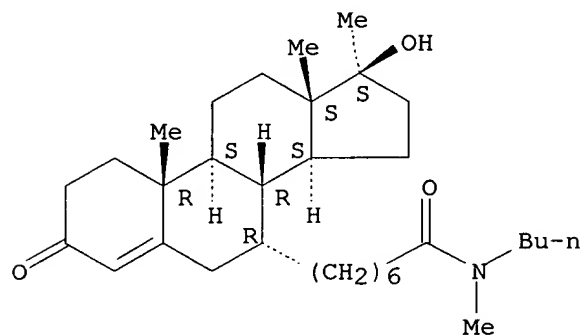
Absolute stereochemistry.



RN 278604-78-7 HCAPLUS

CN Androst-4-ene-7-heptanamide, N-butyl-17-hydroxy-N,17-dimethyl-3-oxo-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

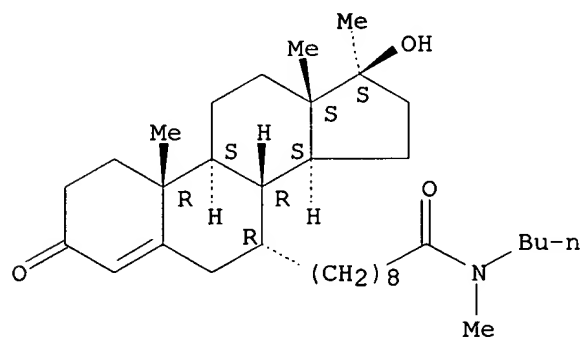
Absolute stereochemistry.



RN 278604-81-2 HCAPLUS

CN Androst-4-ene-7-nonanamide, N-butyl-17-hydroxy-N,17-dimethyl-3-oxo-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

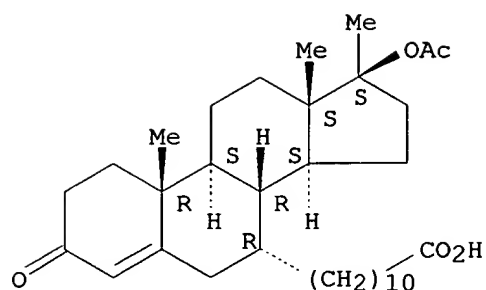
Absolute stereochemistry.



RN 278604-82-3 HCAPLUS

CN Androst-4-ene-7-undecanoic acid, 17-(acetyloxy)-17-methyl-3-oxo-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

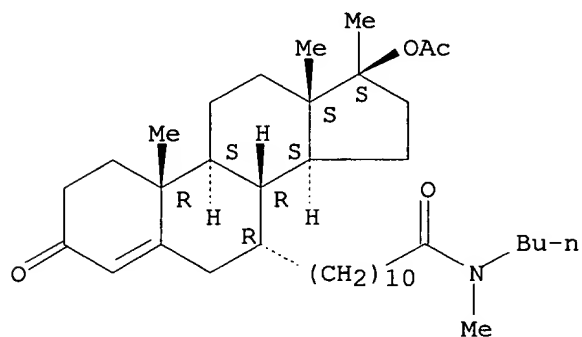
Absolute stereochemistry.



RN 278604-83-4 HCAPLUS

CN Androst-4-ene-7-undecanamide, 17-(acetyloxy)-N-butyl-N,17-dimethyl-3-oxo-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

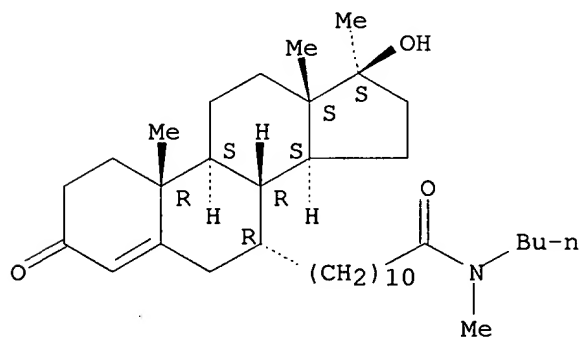
Absolute stereochemistry.



RN 278604-84-5 HCAPLUS

CN Androst-4-ene-7-undecanamide, N-butyl-17-hydroxy-N,17-dimethyl-3-oxo-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

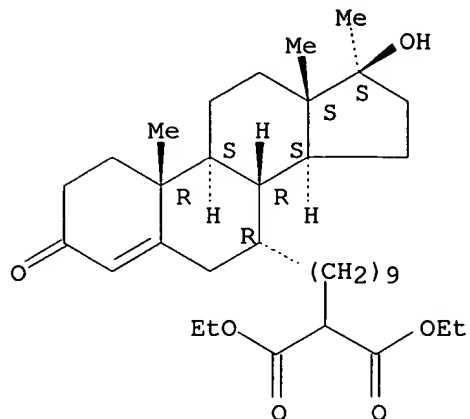
Absolute stereochemistry.



RN 278604-85-6 HCAPLUS

CN Propanedioic acid, [9-[(7.alpha.,17.beta.)-17-hydroxy-17-methyl-3-oxoandrost-4-en-7-yl]nonyl]-, diethyl ester (9CI) (CA INDEX NAME)

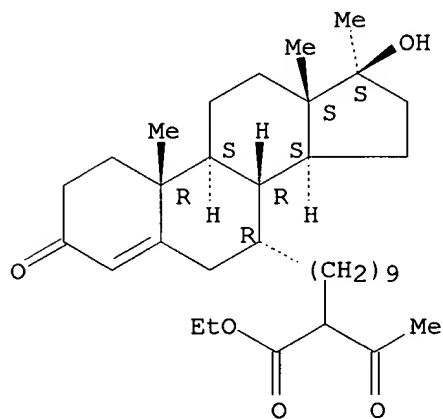
Absolute stereochemistry.



RN 278604-86-7 HCAPLUS

CN Androst-4-ene-7-undecanoic acid, .alpha.-acetyl-17-hydroxy-17-methyl-3-oxo-, ethyl ester, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

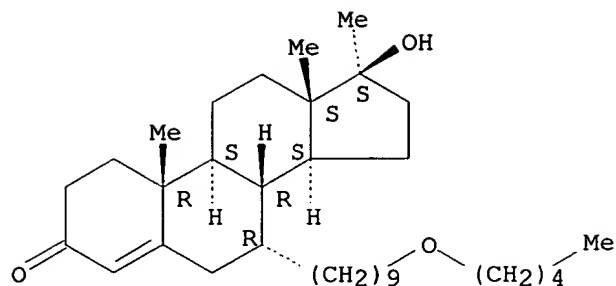
Absolute stereochemistry.



RN 278604-87-8 HCAPLUS

CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[9-(pentyloxy)nonyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

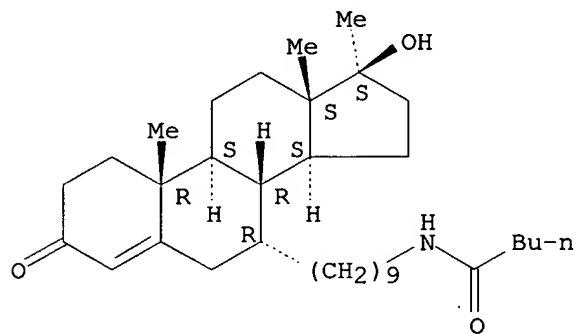
Absolute stereochemistry.



RN 278604-88-9 HCAPLUS

CN Pentanamide, N-[9-[(7.alpha.,17.beta.)-17-hydroxy-17-methyl-3-oxoandrost-4-en-7-yl]nonyl]- (9CI) (CA INDEX NAME)

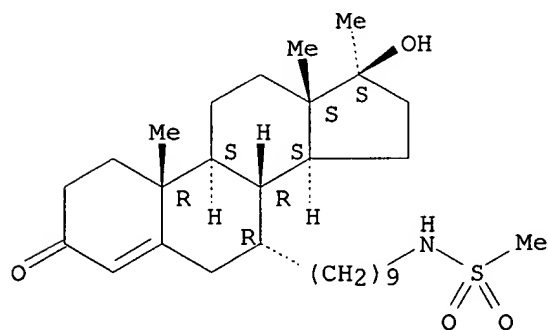
Absolute stereochemistry.



RN 278604-89-0 HCAPLUS

CN Methanesulfonamide, N-[9-[(7.alpha.,17.beta.)-17-hydroxy-17-methyl-3-oxoandrost-4-en-7-yl]nonyl]- (9CI) (CA INDEX NAME)

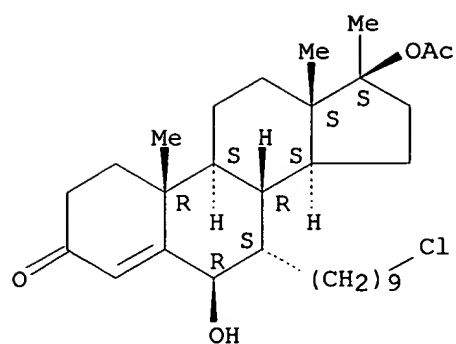
Absolute stereochemistry.



RN 278604-90-3 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-(9-chlorononyl)-6-hydroxy-17-methyl-, (6.beta.,7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

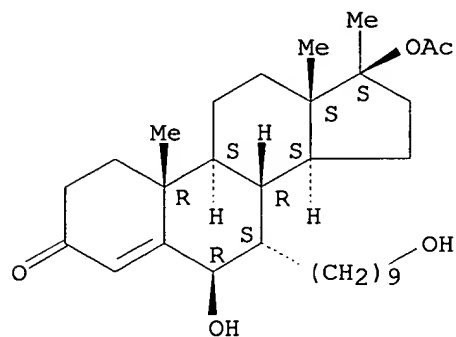
Absolute stereochemistry.



RN 278604-91-4 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-6-hydroxy-7-(9-hydroxynonyl)-17-methyl-, (6.beta.,7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

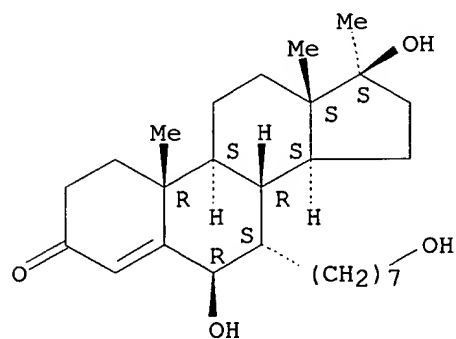
Absolute stereochemistry.



RN 278604-92-5 HCAPLUS

CN Androst-4-en-3-one, 6,17-dihydroxy-7-(7-hydroxyheptyl)-17-methyl-, (6.beta.,7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

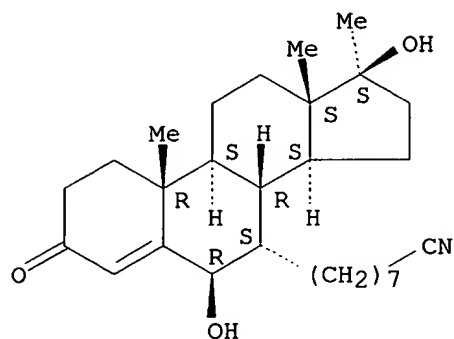


RN 278604-93-6 HCAPLUS

CN Androst-4-ene-7-octanenitrile, 6,17-dihydroxy-17-methyl-3-oxo-, (6.beta.,7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

(6.beta.,7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

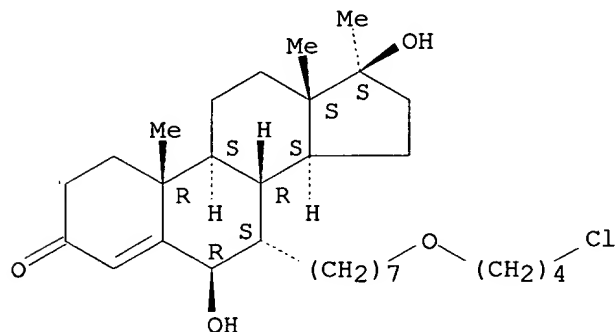
Absolute stereochemistry.



RN 278604-94-7 HCAPLUS

CN Androst-4-en-3-one, 7-[7-(4-chlorobutoxy)heptyl]-6,17-dihydroxy-17-methyl-, (6.beta.,7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:178509 HCAPLUS

DOCUMENT NUMBER: 132:334660

TITLE: Concepts for the syntheses of biotinylated steroids.  
Part I: Testosterone derivatives as immunochemical probesAUTHOR(S): Hauptmann, Hagen; Paulus, Birgit; Kaiser, Thomas;  
Herdtweck, Eberhardt; Huber, Erasmus; Lippa, Peter B.CORPORATE SOURCE: Institute for Organic Chemistry, Universitaet  
Regensburg, Regensburg, D-93053, GermanySOURCE: Bioconjugate Chemistry (2000), 11(2), 239-252  
CODEN: BCCHES; ISSN: 1043-1802

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 132:334660

AB Synthetic strategies for the biotinylation of testosterone (T) at  
positions 3, 7.alpha., 17.alpha., and 19 are described. These T probes



are able to mimic ligand binding and may provide for a better understanding of the biospecific interaction with steroid-binding proteins such as the androgen receptor, anti-steroid antibodies, or steroid-binding serum globulins. For the 7.alpha.- and 17.alpha.-derivs., biotinyl-N-hydroxy-succinimide esters with different types of spacer chains were used. The 3-biotin hydrazone deriv. was produced using N-(.epsilon.-biotinyl)-caproyl hydrazide, whereas for the 19-biotinylation, a biotinyl-1-N-diamino-3,6-dioxaoctane-amide was applied. Key reaction for the biotinylation at position 3 is the oximation of the 3-oxo function. The 17.alpha.-position is accessible by the reaction of the 3-protected 4-androsten-17-epoxide with oxygen in the .beta.-position, followed by nucleophilic ring opening with cyanide which provides the 17.alpha.-cyanomethyl deriv. The key step is the regioselective ketal protection of the 3-oxo function of androst-4-ene-3,17-dione using a stannoxane catalyst. An alternative pathway for the insertion of biotin at the 19-position was established by the synthesis of 17.beta.-hydroxy-androst-4-en-3-one-19-yl carboxymethyl ether. After activation by the carbodiimide method, the compd. reacts with aminoterminal biotin derivs. The copper(I)-catalyzed 1,6 Michael addn. of 17-acetoxy-6,7-dehydro-T leads to 7.alpha.-derivs. by use of .omega.-silyl protected hydroxylalkyl-modified Grignard reagents. A functional group interconversion using the Staudinger reaction transforms the azide function into a primary .omega.-amino group. The abs. configurations of the different biotinylated derivs. were investigated by 1H NMR studies. For the 7.alpha.-biotinylated T series, addnl., an X-ray anal. proved the axial position of the spacer group. This results in a vertical orientation of the biotin moiety toward the .alpha.-face of the planar tetracyclic backbone. Thus, a negligible alteration of the original structure of the upper .beta.-face offers the feasibility of applying the 7.alpha.-derivs. as optimal immunochem. tracers in competitive immunoassays. Biotinylated T derivs. should be also suitable for ligand-binding studies to the androgen receptor or to sex hormone-binding globulin.

IT 134187-54-5P 175479-27-3P 175479-29-5P  
 175479-30-8P 267898-40-8P 267898-41-9P  
 267898-43-1P 267898-45-3P 267898-47-5P  
 267898-48-6P 267898-50-0P 267898-53-3P  
 267898-55-5P 267898-57-7P 267898-59-9P  
 267898-61-3P 267898-63-5P

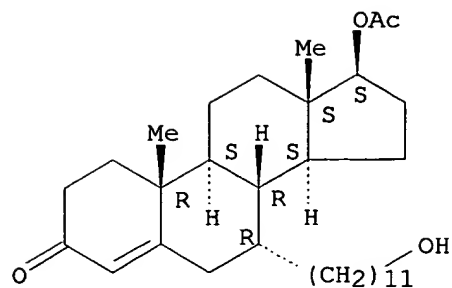
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(syntheses of biotinylated steroids, testosterone derivs. as immunochem. probes)

RN 134187-54-5 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-(11-hydroxyundecyl)-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

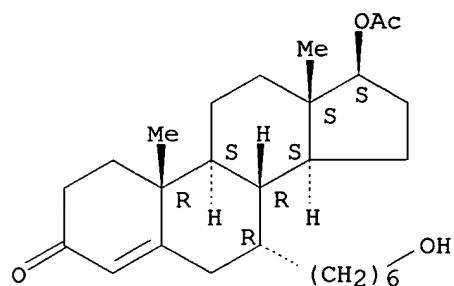
Absolute stereochemistry.



RN 175479-27-3 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-(6-hydroxyhexyl)-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

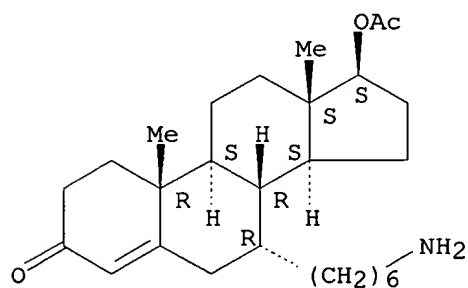
Absolute stereochemistry.



RN 175479-29-5 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-(6-aminoethyl)-, (7.alpha.,17.beta.)-  
(9CI) (CA INDEX NAME)

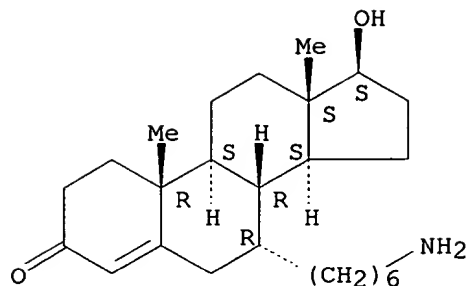
Absolute stereochemistry.



RN 175479-30-8 HCAPLUS

CN Androst-4-en-3-one, 7-(6-aminoethyl)-17-hydroxy-, (7.alpha.,17.beta.)-  
(9CI) (CA INDEX NAME)

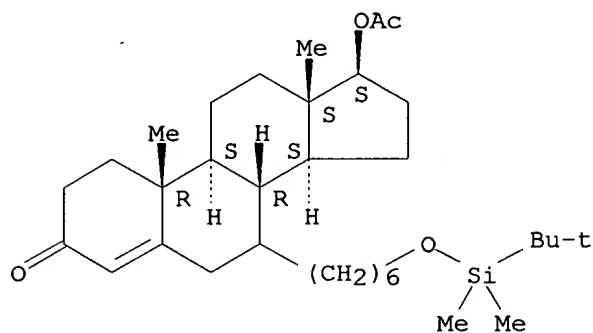
Absolute stereochemistry.



RN 267898-40-8 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-[6-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]hexyl]-, (17.beta.)- (9CI) (CA INDEX NAME)

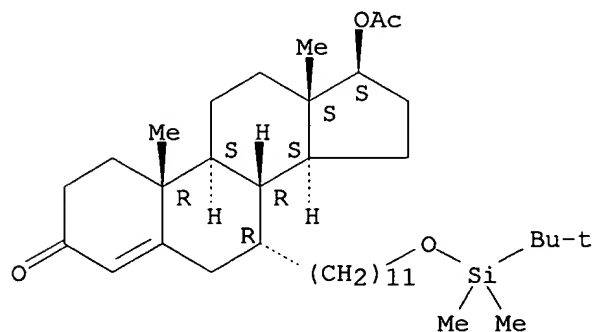
Absolute stereochemistry.



RN 267898-41-9 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-[11-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]undecyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

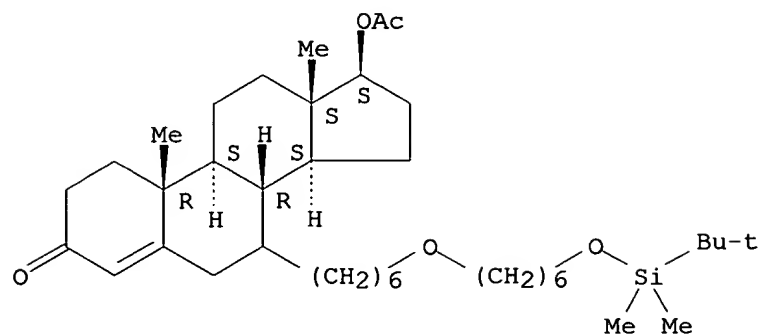


RN 267898-43-1 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-[6-[[[6-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]hexyl]oxy]hexyl]-, (17.beta.)- (9CI) (CA INDEX NAME)

INDEX NAME)

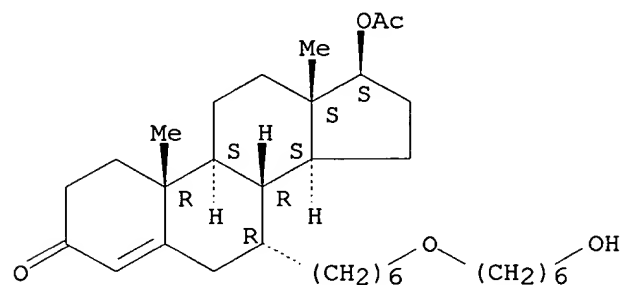
Absolute stereochemistry.



RN 267898-45-3 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-[6-[(6-hydroxyhexyl)oxy]hexyl]-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

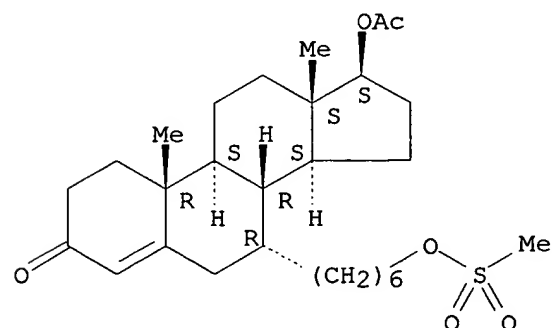
Absolute stereochemistry.



RN 267898-47-5 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-[6-[(methanesulfonyl)oxy]hexyl]-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

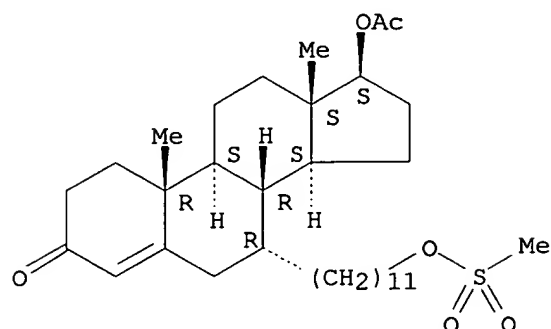
Absolute stereochemistry.



RN 267898-48-6 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-[11-[(methylsulfonyl)oxy]undecyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

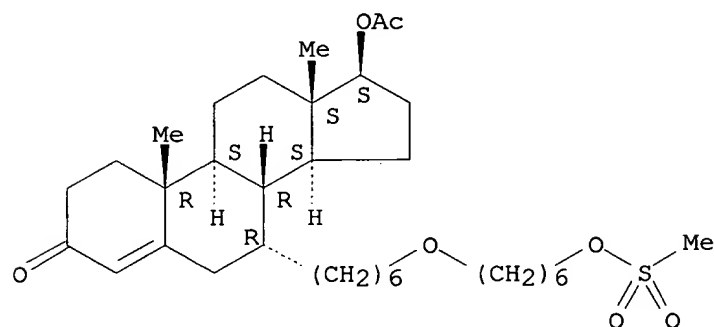
Absolute stereochemistry.



RN 267898-50-0 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-[6-[[6-[(methylsulfonyl)oxy]hexyl]oxy]hexyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

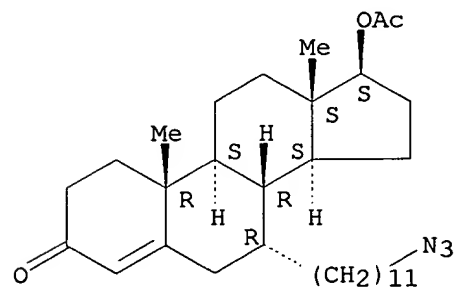
Absolute stereochemistry.



RN 267898-53-3 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-(11-azidoundecyl)-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

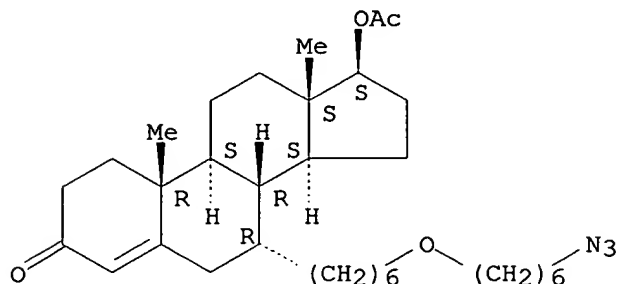
Absolute stereochemistry.



RN 267898-55-5 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-[6-[(6-azidohexyl)oxy]hexyl]-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

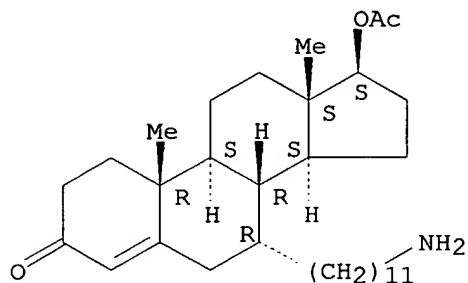
Absolute stereochemistry.



RN 267898-57-7 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-(11-aminoundecyl)-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

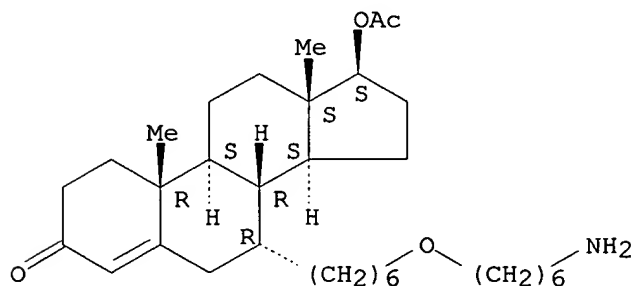
Absolute stereochemistry.



RN 267898-59-9 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-[6-[(6-aminoethyl)oxy]hexyl]-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

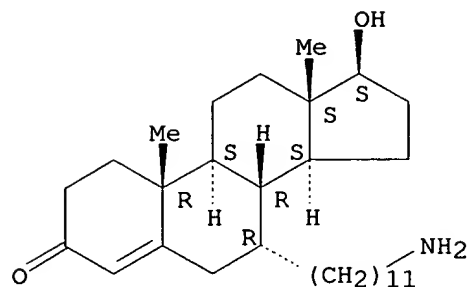
Absolute stereochemistry.



RN 267898-61-3 HCAPLUS

CN Androst-4-en-3-one, 7-(11-aminoundecyl)-17-hydroxy-, (7.alpha.,17.beta.)-  
(9CI) (CA INDEX NAME)

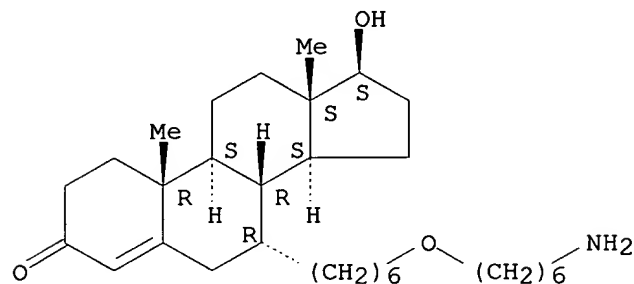
Absolute stereochemistry.



RN 267898-63-5 HCAPLUS

CN Androst-4-en-3-one, 7-[6-[(6-aminohexyl)oxy]hexyl]-17-hydroxy-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



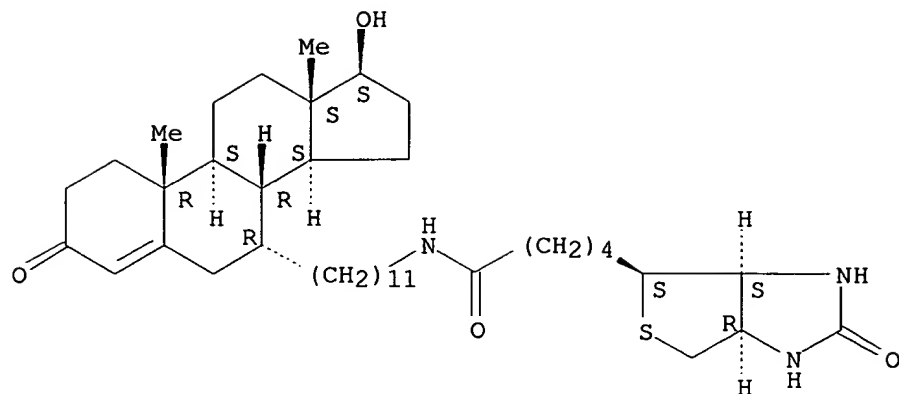
IT 202285-12-9P 267898-52-2P 267898-64-6P  
267898-66-8P 267898-67-9P 267898-68-0P  
267898-86-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(syntheses of biotinylated steroids, testosterone derivs. as  
immunochem. probes)

RN 202285-12-9 HCAPLUS

CN 1H-Thieno[3,4-d]imidazole-4-pentanamide, hexahydro-N-[11-  
[(7.alpha.,17.beta.)-17-hydroxy-3-oxoandrost-4-en-7-yl]undecyl]-2-oxo-,  
(3aS,4S,6aR)- (9CI) (CA INDEX NAME)

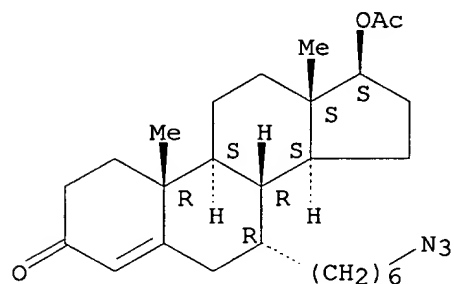
Absolute stereochemistry.



RN 267898-52-2 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-(6-azidoheptyl)-, (7.alpha.,17.beta.)-  
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

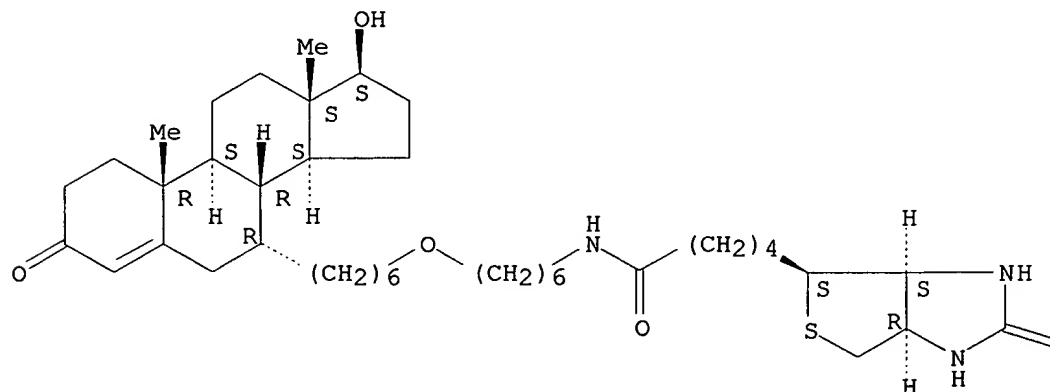


RN 267898-64-6 HCAPLUS

CN 1H-Thieno[3,4-d]imidazole-4-pentanamide, hexahydro-N-[6-[[6-  
[(7.alpha.,17.beta.)-17-hydroxy-3-oxoandrost-4-en-7-yl]hexyl]oxy]hexyl]-2-  
oxo-, (3aS,4S,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





PAGE 1-B

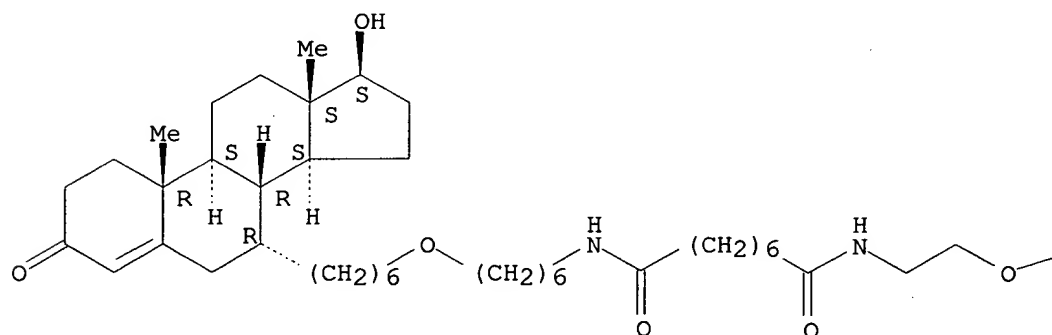
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RN 267898-66-8 HCAPLUS

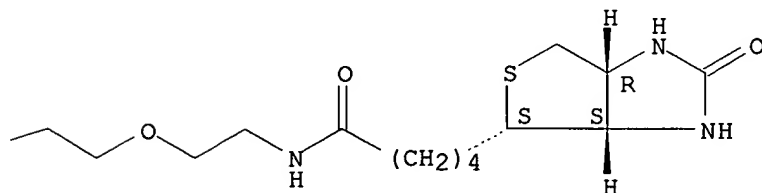
CN Octanediarnide, N-[2-[2-[2-[[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]amino]ethoxy]ethoxy]ethyl]-N'-[6-[[6-[(7.alpha.,17.beta.)-17-hydroxy-3-oxoandrost-4-en-7-yl]hexyl]oxy]hexyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

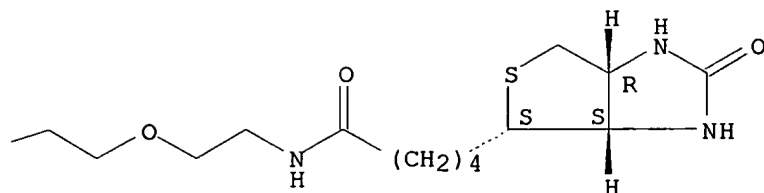
PAGE 1-A



PAGE 1-B



PAGE 1-B

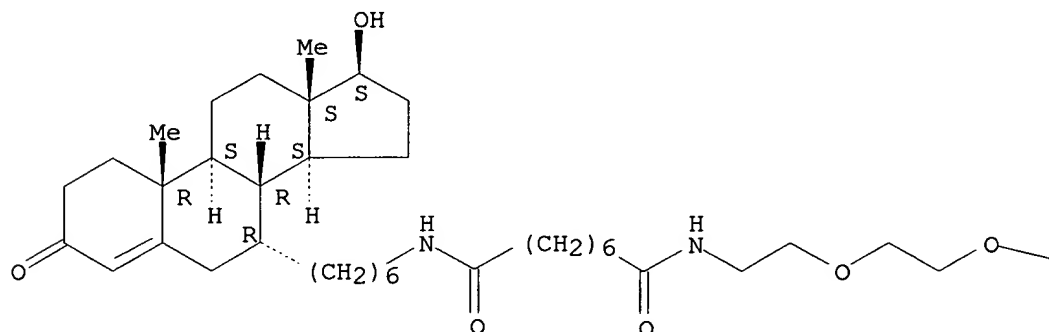


RN 267898-67-9 HCAPLUS

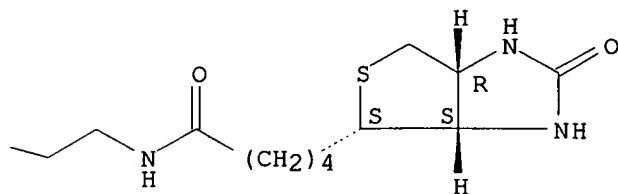
CN Octanediamide, N-[2-[2-[2-[[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]amino]ethoxy]ethoxy]ethyl]-N'-[6-[(7.alpha.,17.beta.)-17-hydroxy-3-oxoandrost-4-en-7-yl]hexyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



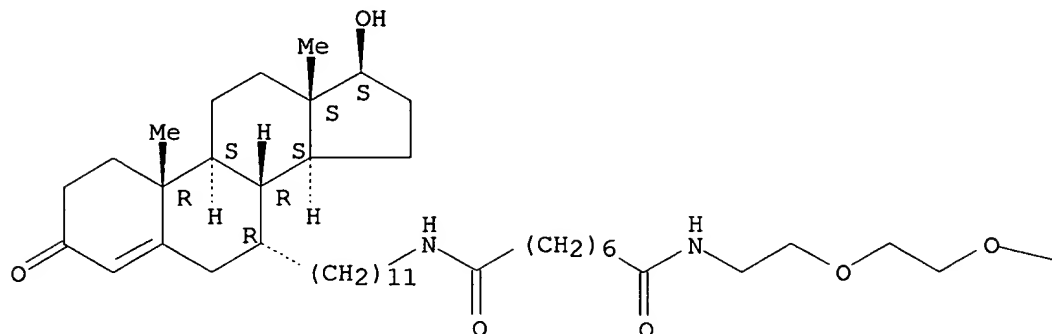
RN 267898-68-0 HCAPLUS

CN Octanediamide, N-[2-[2-[2-[[5-[(3aS,4S,6aR)-hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl]-1-oxopentyl]amino]ethoxy]ethoxy]ethyl]-N'-[11-

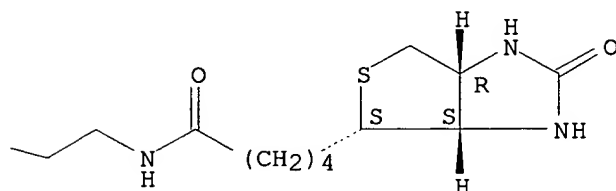
[(7.alpha.,17.beta.)-17-hydroxy-3-oxoandrost-4-en-7-yl]undecyl]- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



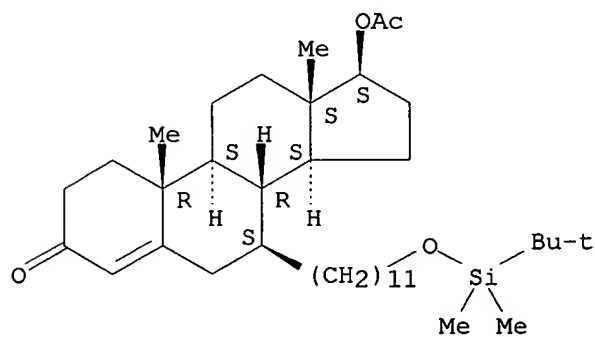
PAGE 1-B



RN 267898-86-2 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-[11-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]undecyl]-, (7.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 77 THERE ARE 77 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:26600 HCAPLUS

DOCUMENT NUMBER: 128:136570

TITLE: 7.alpha.-Biotinylated testosterone derivatives as tracers for a competitive chemiluminescence immunoassay of testosterone in serum

AUTHOR(S): Lippa, Peter; Bruckner, Christine; Schwab, Ingrid; Hauck, Sabine; Schmidmayr, Stefan; Birkmayer, Christian; Paulus, Birgit; Hauptmann, Hagen

CORPORATE SOURCE: Institute of Clinical Chemistry and Pathobiochemistry, Klinikum rechts der Isar, Technical University Munich, Munich, D-81675, Germany

SOURCE: Clinical Chemistry (Washington, D. C.) (1997), 43(12), 2345-2352

CODEN: CLCHAU; ISSN: 0009-9147

PUBLISHER: American Association for Clinical Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Ring core-biotinylated testosterone tracers were synthesized with bridges of three different lengths connecting the biotin moiety to the steroid core (7.alpha.-Cn-Bio-T, n = 3, 6, or 11). Together with a position 7-specific polyclonal anti-testosterone antibody, we used the 7.alpha.-C11-Bio-T tracer to develop a novel, labeled-hapten competitive immunoassay for total testosterone in serum. (The C3 and C6 tracers proved to be not suitable for analogous immunoassays.). Enhanced chemiluminescence signal was generated by use of a second immobilized antibody and a streptavidin-horseradish peroxidase conjugate. The measuring range of the assay is 0.2-20.0 nmol/L, linearity of serial dilns. can be demonstrated, the lower detection limit is 0.125 nmol/L, and the interassay imprecisions are 13-16%. Accuracy detns. in mass spectrometry-controlled ref. specimens showed a mean recovery of 95%. In addn., the assay shows low cross-reactivities, demonstrating the favorable specificity of the combination of a "nearly native" tracer with a position analog antibody. The optimized steric structure and the long spacer arm of the biotinylated testosterone tracer make this chemiluminescence assay well-suited for measuring total testosterone concn. in serum.

IT 175479-31-9P 202285-12-9P

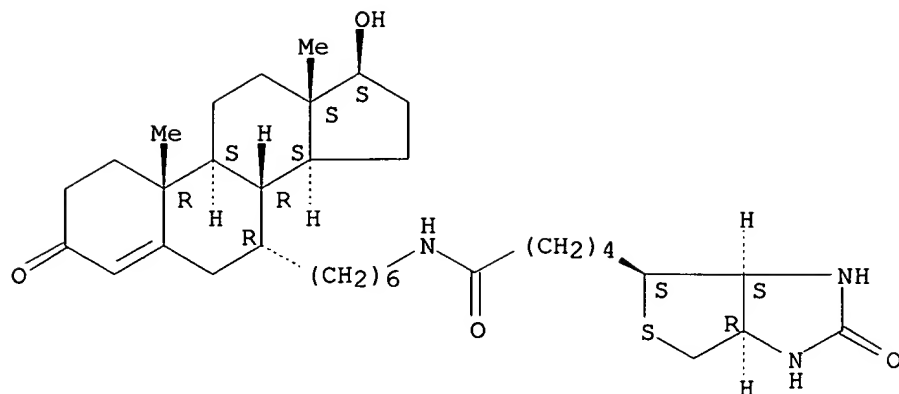
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)

(7.alpha.-biotinylated testosterone derivs. as tracers for a competitive chemiluminescence immunoassay of testosterone in serum)

RN 175479-31-9 HCAPLUS

CN 1H-Thieno[3,4-d]imidazole-4-pentanamide, hexahydro-N-[6-[(7.alpha.,17.beta.)-17-hydroxy-3-oxoandrost-4-en-7-yl]hexyl]-2-oxo-, [3aS-(3a.alpha.,4.beta.,6a.alpha.)]- (9CI) (CA INDEX NAME)

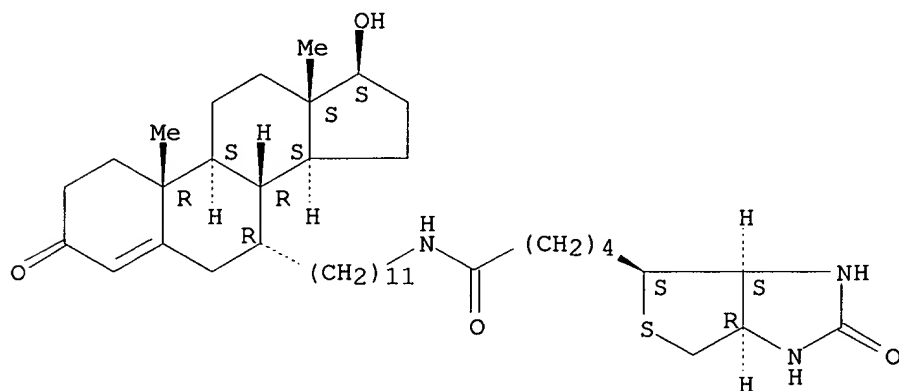
Absolute stereochemistry.



RN 202285-12-9 HCAPLUS

CN 1H-Thieno[3,4-d]imidazole-4-pentanamide, hexahydro-N-[11-  
[(7.alpha.,17.beta.)-17-hydroxy-3-oxoandrost-4-en-7-yl]undecyl]-2-oxo-,  
(3aS,4S,6aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:280333 HCAPLUS

DOCUMENT NUMBER: 124:307782

TITLE: Synthesis of 17.beta.-Hydroxyandrost-4-en-3-one-  
7.alpha.-(Biotinyl-6-N-hexylamide), a Conjugate useful  
for Affinity Chromatography and for Testosterone  
Immunoassays

AUTHOR(S): Luppa, Peter; Hauck, Sabine; Schwab, Ingrid;  
Birkmayer, Christian; Hauptmann, Hagen

CORPORATE SOURCE: Institute for Clinical Chemistry and  
Pathobiochemistry, Technical University Munich,  
Munich, D-81675, Germany

SOURCE: Bioconjugate Chemistry (1996), 7(3), 332-337  
CODEN: BCCHE; ISSN: 1043-1802

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The authors describe the synthesis of 17.beta.-hydroxyandrost-4-en-3-one-7.alpha.-(biotinyl-6-N-hexylamide) from 17.beta.-hydroxyandrost-4-en-3-one (testosterone) via copper-catalyzed 1,6 Michael addn. of a 6-(tert-butyldimethylsilyloxyhexyl) chain to 6-dehydrotestosterone 17.beta.-acetate. After chromatog. sepn. of the 7.alpha.-isomer from the .alpha./.beta. mixt. and cleavage of the silyl ether, the alc. was oxidized to the 6-hexanal side chain and then subjected to reductive amination. The resulting primary amine is easily biotinylated using biotinyl-N-hydroxysuccinimide ester. The overall yield for the epimeric 7.alpha.-end product was 30%. The abs. configurations of the epimers were investigated by 1H NMR studies by the nuclear Overhauser effect. The authors introduced a biotin label to the testosterone mol. at ring position 7 in compliance with Landsteiner's principle, which states that antibody specificity is directed primarily at that portion of the hapten furthest from the functional group linking it to the carrier protein. Thus, this negligible alteration in comparison to the structure of the resp. testosterone hapten used to elicit antibodies offers the feasibility of applying the testosterone deriv. as an optimal immunoabsorbent in affinity chromatog. The 7.alpha.-biotinylated testosterone was used to obtain active antitestosterone antibodies from a specific antiserum by affinity chromatog. This was achieved by attaching the biotinylated testosterone to agarose-coupled streptavidin beads. Accordingly, a 3H-testosterone-binding test demonstrated a 20-fold increase in affinity of the purified antibody to the steroid compared to the original antiserum, and a recovery of >80% could be obtained. The antitestosterone antibody, obtained by that method, is an effective component for use in a competitive immunoassay for testosterone in human sera. An assay configuration is conceivable with the same 7.alpha.-biotinylated testosterone employed as tracer in combination with a streptavidin-linked reporter enzyme.

IT 175479-24-0P 175479-25-1P 175479-27-3P

175479-28-4P 175479-29-5P 175479-30-8P

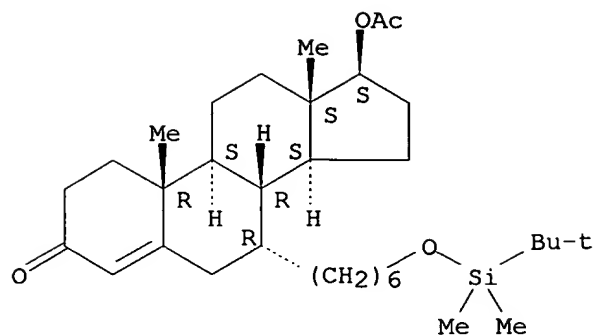
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of 17.beta.-hydroxyandrost-4-en-3-one-7.alpha.-(biotinyl-6-N-hexylamide), a conjugate useful for affinity chromatog. and for testosterone immunoassays)

RN 175479-24-0 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-[6-[[[1,1-dimethylethyl]dimethylsilyl]oxy]hexyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

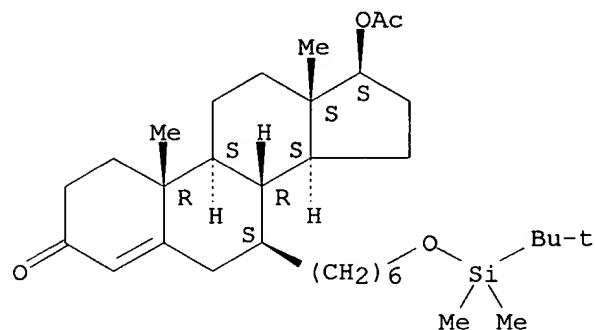
Absolute stereochemistry.



RN 175479-25-1 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-[6-[(1,1-dimethylethyl)dimethylsilyl]oxy]hexyl]-, (7.beta.,17.beta.)- (9CI) (CA INDEX NAME)

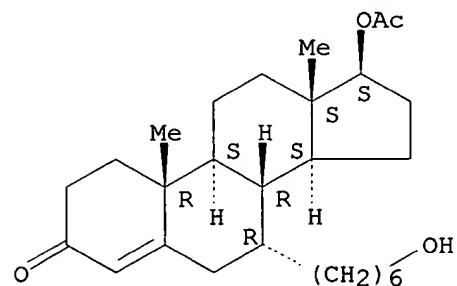
Absolute stereochemistry.



RN 175479-27-3 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-(6-hydroxyhexyl)-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

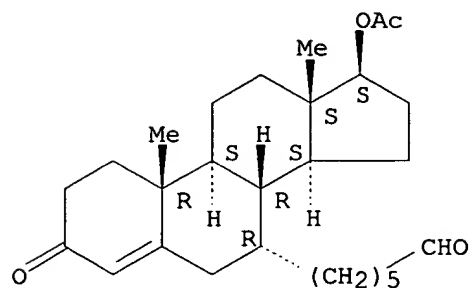
Absolute stereochemistry.



RN 175479-28-4 HCAPLUS

CN Androst-4-ene-7-hexanal, 17-(acetyloxy)-3-oxo-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

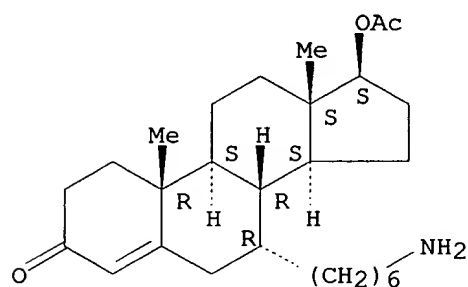
Absolute stereochemistry.



RN 175479-29-5 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-(6-aminohexyl)-, (7.alpha.,17.beta.)-(9CI) (CA INDEX NAME)

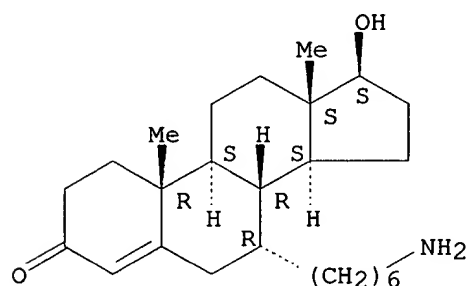
Absolute stereochemistry.



RN 175479-30-8 HCAPLUS

CN Androst-4-en-3-one, 7-(6-aminohexyl)-17-hydroxy-, (7.alpha.,17.beta.)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **175479-31-9P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(synthesis of 17.beta.-hydroxyandrost-4-en-3-one-7.alpha.-(biotinyl-6-N-hexylamide), a conjugate useful for affinity chromatog. and for testosterone immunoassays)

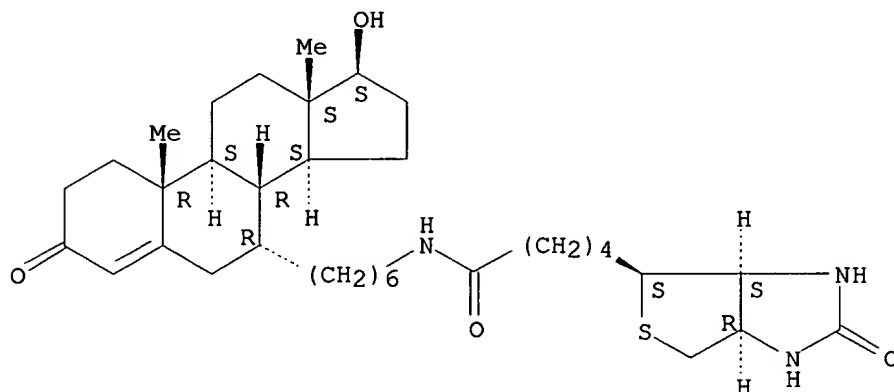
RN 175479-31-9 HCAPLUS

CN 1H-Thieno[3,4-d]imidazole-4-pentanamide, hexahydro-N-[6-



[(7.alpha.,17.beta.)-17-hydroxy-3-oxoandrost-4-en-7-yl]hexyl]-2-oxo-,  
[3aS-(3a.alpha.,4.beta.,6a.alpha.)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1991:574681 HCAPLUS

DOCUMENT NUMBER: 115:174681

TITLE: Preparation of steroid enzyme inhibitors for treatment of benign prostatic hyperplasia

INVENTOR(S): Labrie, Fernand

PATENT ASSIGNEE(S): Endorecherche Inc., Can.

SOURCE: PCT Int. Appl., 75 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 8

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9100731	A1	19910124	WO 1990-CA210	19900705
W: AT, AU, BB, BG, BR, CA, CH, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MC, MG, MW, NL, NO, RO, SD, SE, SU				
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CA 2062973	AA	19910108	CA 1990-2062973	19900705
AU 9058545	A1	19910206	AU 1990-58545	19900705
AU 643445	B2	19931118		
EP 480950	A1	19920422	EP 1990-909598	19900705
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HU 60138	A2	19920828	HU 1992-47	19900705
JP 04506798	T2	19921126	JP 1990-509262	19900705
JP 3332377	B2	20021007		
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ES 2133270	T3	19990916	ES 1990-909598	19900705
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EP 943328 A3 19991208  
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 IL 94990 A1 19970110 IL 1990-94990 19900706  
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 AU 668434 B2 19960502  
 US 5595985 A 19970121 US 1993-167450 19931215  
 US 5817649 A 19981006 US 1995-476933 19950607  
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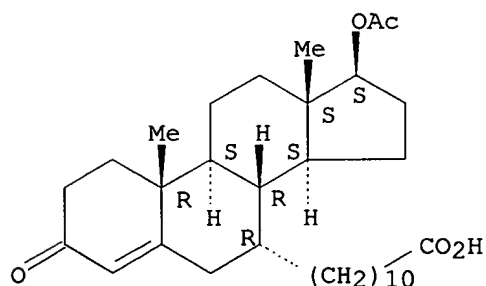
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 US 1989-322154 B2 19890310  
 EP 1990-909598 A3 19900705  
 EP 1998-104849 A3 19900705  
 JP 1990-509262 A3 19900705  
 WO 1990-CA210 A 19900705  
 US 1992-925883 B1 19920806  
 US 1993-167450 A3 19931215  
 AU 1996-46606 A3 19960220  
 AU 1997-46772 A3 19971128

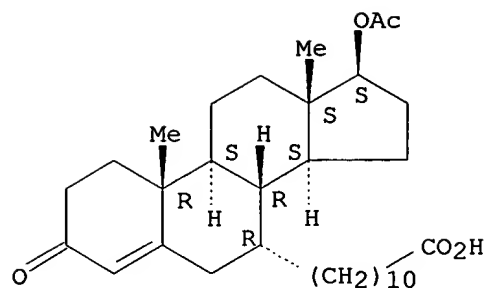
AB A method of preventing and/or treating benign prostatic hyperplasia (BPH) in humans or warm-blooded animals comprises orally or parenterally administering .gtoreq.2 compds. selected from a 5.alpha.-reductase inhibitor, an antiestrogen, an aromatase inhibitor, a 17.beta.-hydroxy steroid dehydrogenase (17.beta.-HSD) inhibitor, and further an antiandrogen and an LH-RH agonist or antagonist. A 5-reductase inhibitor is 4-MA or MK-906; an antiestrogen is (Z)-2-[4-(1,2-diphenyl-1-butenyl)phenoxy]-N,N-dimethylethanamine, EM 139 (prepn. given), EM 142, etc.; an aromatase inhibitor is FCE 24304 or 4-hydroxyandrostenedione; and an antiandrogen is flutamide. EM 139 was prepd. starting from 19-nortestosterone by protection, addn. with undecanol by Grignard reaction, dehydrogenation and deprotection, oxidn. and amidation with butylmethylamine, enol esterifying, and chlorination.

IT **91454-67-0P 134187-54-5P 134187-55-6P 134187-56-7P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (prepn. and reaction of, in prepn. of prostatic hyperplasia drug)

RN 91454-67-0 HCAPLUS  
 CN Androst-4-ene-7-undecanoic acid, 17-(acetyloxy)-3-oxo-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

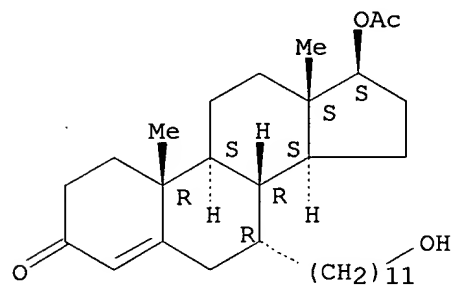




RN 134187-54-5 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-(11-hydroxyundecyl)-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

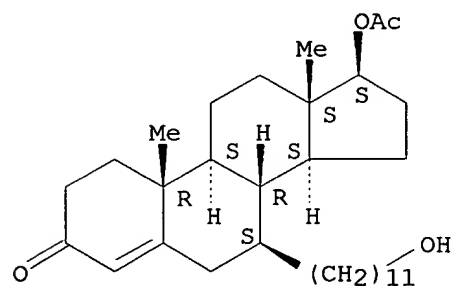
Absolute stereochemistry.



RN 134187-55-6 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-(11-hydroxyundecyl)-,  
(7.beta.,17.beta.)- (9CI) (CA INDEX NAME)

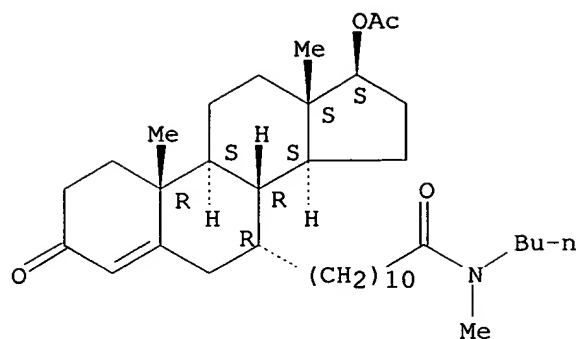
Absolute stereochemistry.



RN 134187-56-7 HCAPLUS

CN Androst-4-ene-7-undecanamide, 17-(acetyloxy)-N-butyl-N-methyl-3-oxo-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



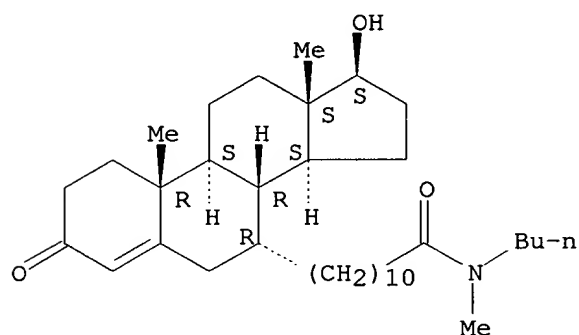
IT 134187-57-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, for prostatic hyperplasia treatment)

RN 134187-57-8 HCAPLUS

CN Androst-4-ene-7-undecanamide, N-butyl-17-hydroxy-N-methyl-3-oxo-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1991:485452 HCAPLUS

DOCUMENT NUMBER: 115:85452

TITLE: Preparation of steroidal enzyme inhibitors for  
treatment of prostate cancer

INVENTOR(S): Labrie, Fernand

PATENT ASSIGNEE(S): Endorecherche Inc., Can.

SOURCE: PCT Int. Appl., 102 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 8

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9100733	A1	19910124	WO 1990-CA212	19900705
W: AT, AU, BB, BG, BR, CA, CH, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MC, MG, MW, NL, NO, RO, SD, SE, SU				

RW: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE

CA 2062792	AA	19910108	CA 1990-2062792	19900705
AU 9058516	A1	19910206	AU 1990-58516	19900705
HU 60139	A2	19920828	HU 1992-48	19900705
JP 04506799	T2	19921126	JP 1990-509263	19900705
JP 3350048	B2	20021125		
EP 595796	A1	19940511	EP 1990-909601	19900705
EP 595796	B1	20030115		

R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE

AT 230994	E	20030215	AT 1990-909601	19900705
ES 2189784	T3	20030716	ES 1990-909601	19900705
ZA 9005313	A	19920226	ZA 1990-5313	19900706
IL 94991	A1	19991130	IL 1990-94991	19900706
US 5372996	A	19941213	US 1992-963278	19921019
US 5593981	A	19970114	US 1993-98607	19930910
AU 9463425	A1	19940721	AU 1994-63425	19940530
AU 665311	B2	19951221		
US 5610150	A	19970311	US 1995-472512	19950607
AU 760232	B2	20030508	AU 2000-20637	20000303
AU 762751	B2	20030703	AU 2000-34056	20000512
AU 2000034056	A5	20000720		

PRIORITY APPLN. INFO.:

	US 1989-376710	A	19890707
	US 1989-322154	B2	19890310
	WO 1990-CA212	A	19900705
	US 1992-963278	A3	19921019
	US 1993-98607	A3	19930910
	AU 1996-46606	A3	19960220
	AU 1997-46772	A3	19971128

OTHER SOURCE(S): MARPAT 115:85452

AB A method of treatment of androgen-related diseases (e.g. prostate cancer) in male humans or warm-blooded animals comprises administering novel antiandrogens and/or novel sex steroid biosynthesis inhibitors as part of a combination therapy. Sex steroid biosynthesis inhibitors, esp. those capable of inhibiting conversion of dehydroepiandrosterone or 4-androstenedione to natural sex steroids (and testosterone into dihydrotestosterone) in peripheral tissues, are used in combination with antiandrogens usually after blockade of testicular hormonal secretions. Antiestrogens can also be part of the combination therapy. Pharmaceutical comps. and 2-, 3-, 4-, and 5-component kits are useful for such combination treatment. EM139 (I) was prepd. starting from 19-nortestosterone by protection, addn. to undecanol by Grignard reaction, dehydrogenation and deprotection, oxidn. and amidation with BuNHMe, acetylenolation, and chlorination.

IT **91454-67-0P 134187-54-5P 134187-55-6P 134187-56-7P**

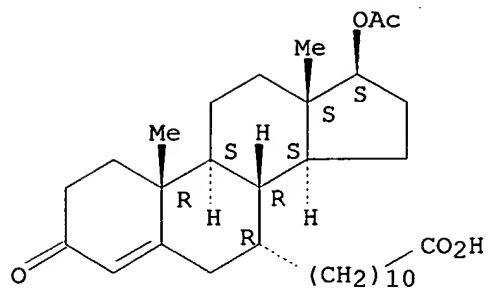
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction of, in prepn. of drug for prostate cancer treatment)

RN 91454-67-0 HCAPLUS

CN Androst-4-ene-7-undecanoic acid, 17-(acetyloxy)-3-oxo-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

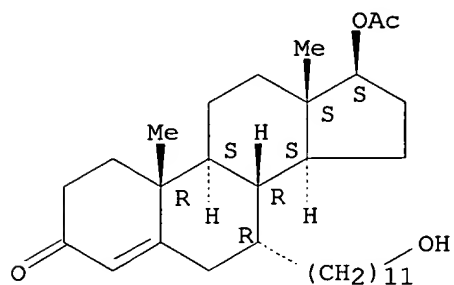
Absolute stereochemistry.



RN 134187-54-5 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-(11-hydroxyundecyl)-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

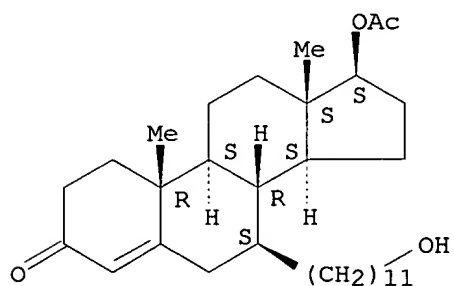
Absolute stereochemistry.



RN 134187-55-6 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-(11-hydroxyundecyl)-,  
(7.beta.,17.beta.)- (9CI) (CA INDEX NAME)

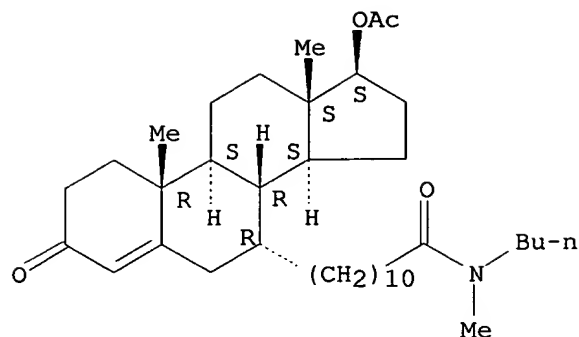
Absolute stereochemistry.



RN 134187-56-7 HCAPLUS

CN Androst-4-ene-7-undecanamide, 17-(acetyloxy)-N-butyl-N-methyl-3-oxo-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



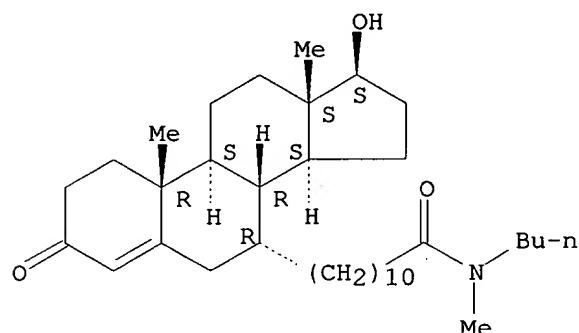
IT 134187-57-8P, EM 101

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, for prostate cancer treatment)

RN 134187-57-8 HCAPLUS

CN Androst-4-ene-7-undecanamide, N-butyl-17-hydroxy-N-methyl-3-oxo-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1991:472016 HCAPLUS

DOCUMENT NUMBER: 115:72016

TITLE: Preparation of .omega.-(androstenonyl)alkynoates and  
analogs as antiandrogenic agents

INVENTOR(S): Labrie, Fernand; Merand, Yves

PATENT ASSIGNEE(S): Endorecherche Inc., Can.

SOURCE: PCT Int. Appl., 73 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 8

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9100732	A1	19910124	WO 1990-CA211	19900705
W: AT, AU, BB, BG, BR, CA, CH, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MC, MG, MW, NL, NO, RO, SD, SE, SU				

RW: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE  
 CA 2063378 AA 19910108 CA 1990-2063378 19900705  
 AU 9058560 A1 19910206 AU 1990-58560 19900705  
 EP 485392 A1 19920520 EP 1990-909608 19900705  
 EP 485392 B1 19980909

R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE  
 HU 60280 A2 19920828 HU 1992-49 19900705  
 JP 04506797 T2 19921126 JP 1990-509137 19900705  
 JP 2959839 B2 19991006  
 AT 170753 E 19980915 AT 1990-909608 19900705  
 ES 2121570 T3 19981201 ES 1990-909608 19900705  
 ZA 9005311 A 19920226 ZA 1990-5311 19900706  
 IL 94992 A1 19980104 IL 1990-94992 19900706  
 AU 9467481 A1 19940908 AU 1994-67481 19940714  
 US 6110906 A 20000829 US 1994-279262 19940721  
 AU 9725598 A1 19970904 AU 1997-25598 19970618  
 AU 692411 B2 19980604  
 AU 760232 B2 20030508 AU 2000-20637 20000303  
 AU 762751 B2 20030703 AU 2000-34056 20000512  
 AU 2000034056 A5 20000720

## PRIORITY APPLN. INFO.:

US 1989-376696 A 19890707  
 US 1989-322154 A2 19890310  
 WO 1990-CA211 A 19900705  
 US 1992-972883 B1 19921105  
 AU 1996-46606 A3 19960220  
 AU 1997-46772 A3 19971128

## OTHER SOURCE(S): MARPAT 115:72016

AB The title compds. [I; A = CH, CH<sub>2</sub>, O; B = CH, CH<sub>2</sub>, N, NH; R<sub>6</sub>-R<sub>9</sub>, R<sub>11</sub>, R<sub>12</sub> = H, Z<sub>1</sub>m(XZ<sub>2</sub>n)xLG; R<sub>10</sub>, R<sub>13</sub> = H, alkyl; L = alkylene, CONH, O, S, NH, CS<sub>2</sub>, etc.; G = H, alkenyl, alkynyl (un)substituted (cyclo)alkyl; LG = N-contg. heterocyclyl; X = O, S, NH, CH<sub>2</sub>, CO<sub>2</sub>, CONH, etc.; Z<sub>1</sub>, Z<sub>2</sub> = (fluoro)alkylene, -alkenylene, -alkynylene, -phenylene; m, n = 0, 1; x = 0-6] were prepd. Thus, ethisterone was diprotected and the product treated with BuLi and I(CH<sub>2</sub>)<sub>10</sub>I to give, after deprotection, title compd. II which gave .apprx.50% inhibition of 17.β.-hydroxysteroid dehydrogenase at .apprx.35 .μM in vitro.

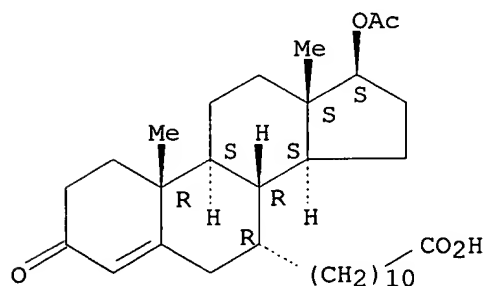
IT **91454-67-0P 134187-54-5P 134187-55-6P 134187-56-7P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (prepn. and reaction of, in prepn. of antiandrogenics)

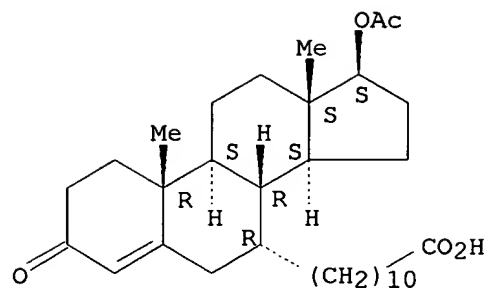
RN 91454-67-0 HCAPLUS

CN Androst-4-ene-7-undecanoic acid, 17-(acetyloxy)-3-oxo-,  
 (7.α.,17.β.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



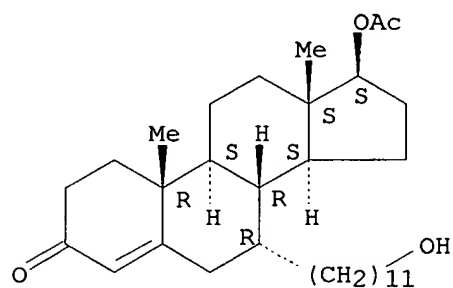




RN 134187-54-5 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-(11-hydroxyundecyl)-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

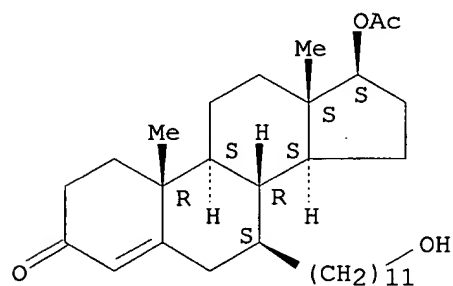
Absolute stereochemistry.



RN 134187-55-6 HCAPLUS

CN Androst-4-en-3-one, 17-(acetyloxy)-7-(11-hydroxyundecyl)-,  
(7.beta.,17.beta.)- (9CI) (CA INDEX NAME)

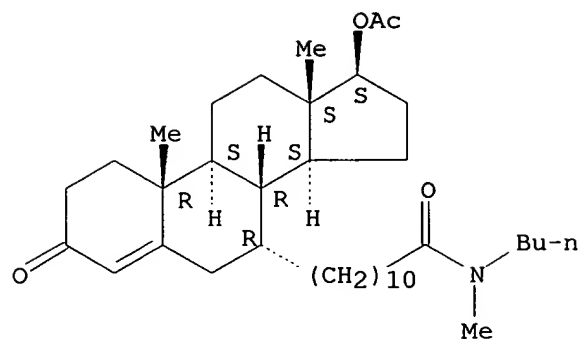
Absolute stereochemistry.



RN 134187-56-7 HCAPLUS

CN Androst-4-ene-7-undecanamide, 17-(acetyloxy)-N-butyl-N-methyl-3-oxo-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



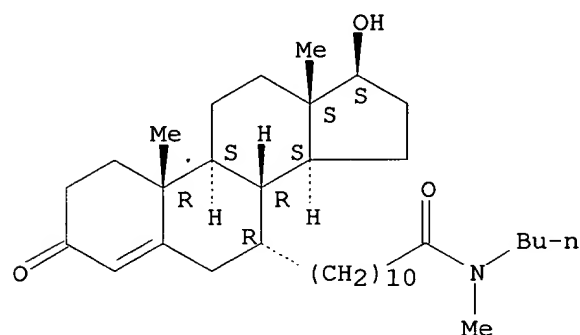
IT 134187-57-8P 134187-58-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, as antiandrogenic)

RN 134187-57-8 HCAPLUS

CN      Androst-4-ene-7-undecanamide, N-butyl-17-hydroxy-N-methyl-3-oxo-,  
           (7.alpha.,17.beta.)- (9CI)    (CA INDEX NAME)

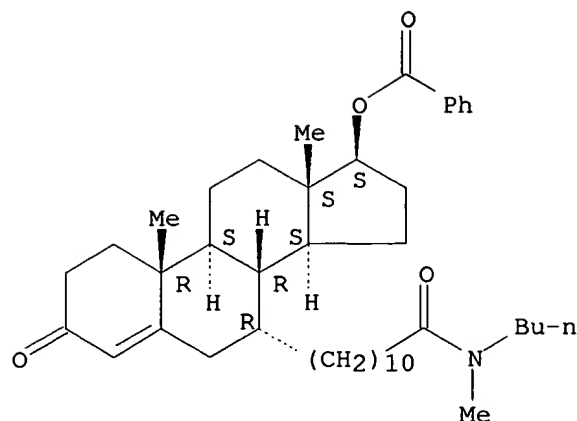
Absolute stereochemistry.



RN 134187-58-9 HCAPLUS

CN    Androst-4-ene-7-undecanamide, 17-(benzoyloxy)-N-butyl-N-methyl-3-oxo-,  
 (7.alpha.,17.beta.)- (9CI)    (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1984:486527 HCAPLUS

DOCUMENT NUMBER: 101:86527

TITLE: Synthesis and evaluation of immobilized androgens for affinity chromatography in the purification of nuclear androgen receptor

AUTHOR(S): De Larminat, Marie Anne; Bruchovsky, Nicholas; Rennie, Paul S.; Lee, Sing Ping; Tertzakian, Gerald

CORPORATE SOURCE: Dep. Cancer Endocrinol., Cancer Control Agency of British Columbia, Vancouver, BC, V5Z 3J3, Can.

SOURCE: Prostate (New York, NY, United States) (1984), 5(2), 123-40

CODEN: PRSTDS; ISSN: 0270-4137

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Seven biospecific adsorbents contg. immobilized androgens were synthesized: dihydrotestosterone-17.beta.-succinyl agarose, and both the unsubstituted and the 17.beta.-acetyl derivs. of dihydrotestosterone-7.alpha.-undecanoyl agarose, testosterone-7.alpha.-undecanoyl agarose, and 19-nortestosterone-7.alpha.-undecanoyl agarose. The retention capacities for nuclear androgen receptor were generally between 40-80% with little variation in reproducibility; the amt. of binding was greatest with dihydrotestosterone-17.beta.-succinyl agarose and dihydrotestosterone-17.beta.-acetoxy-7.alpha.-undecanoyl agarose. Rapid flow rates were obtained with all gels, and no tendency for decompn. was obsd. over a period of 1 yr. Factors that affected retention included the concn. of immobilized androgen, length of the linker arm, occupation of receptor sites, interval of contact with the gel, and temp. of incubation. Chem. dissocn. of androgens from androgen receptor complexes with 0.2 mM mersalyl increased the retention of receptor by dihydrotestosterone-17.beta.-succinyl agarose. Two eluants showed promise for the dissocn. of gel-bound receptor: (1) 0.2 mM mersalyl in the presence of 1.5 mg/mL of ovalbumin; (2) 10% DMF-H2O contg. 30 .mu.M [1,2-3H]dihydrotestosterone and 0.5 M Na thiocyanate.

IT 59287-27-3D, reaction products with Affi-gel 102

91454-67-0D, reaction products with Affi-gel 102

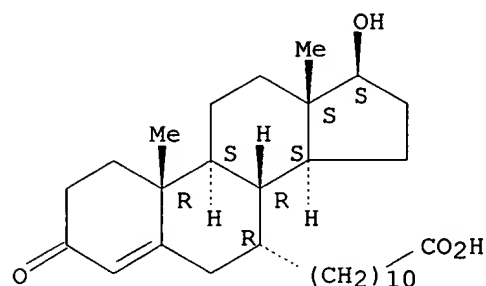
RL: ANST (Analytical study)

(androgen receptor binding by)

RN 59287-27-3 HCAPLUS

CN Androst-4-ene-7-undecanoic acid, 17-hydroxy-3-oxo-, (7.alpha.,17.beta.)-  
(9CI) (CA INDEX NAME)

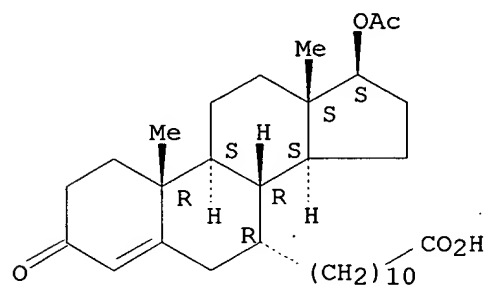
Absolute stereochemistry.



RN 91454-67-0 HCAPLUS

CN Androst-4-ene-7-undecanoic acid, 17-(acetyloxy)-3-oxo-,  
(7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1976:178141 HCAPLUS

DOCUMENT NUMBER: 84:178141

TITLE: Testosterone-derived haptens and their use in  
preparing antigens

INVENTOR(S): Pierdet, Andre; Coussediere, Daniel

PATENT ASSIGNEE(S): Roussel-UCLAF, Fr.

SOURCE: Ger. Offen., 28 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2529969	A1	19760122	DE 1975-2529969	19750704
FR 2277082	A1	19760130	FR 1974-23281	19740704
SE 7507353	A	19760105	SE 1975-7353	19750626
US 3975413	A	19760817	US 1975-592619	19750702
BE 830987	A1	19760105	BE 1975-157970	19750703

DK 7503010	A	19760105	DK 1975-3010	19750703
AU 7582706	A1	19770106	AU 1975-82706	19750703
ES 439100	A1	19770616	ES 1975-439100	19750703
CA 1046502	A1	19790116	CA 1975-230658	19750703
AT 348157	B	19790212	AT 1975-5141	19750703
NL 7507994	A	19760106	NL 1975-7994	19750704
JP 51034144	A2	19760323	JP 1975-81993	19750704
BR 7504242	A	19760706	BR 1975-5432	19750704
ZA 7504298	A	19760825	ZA 1975-4298	19750704
AT 7707904	A	19791115	AT 1977-7904	19771104
AT 357277	B	19800625		

## PRIORITY APPLN. INFO.:

FR 1974-23281	19740704
AT 1975-5141	19750703

AB Testosterone-specific haptens were prepd. by derivitizing the parent steroid at ring positions 7 and 11. Thus, derivs. synthesized were: 7-carboxymethoxyimino-, 11.alpha.- and .beta.-hemiterephthaloyloxy-, 11.beta.-hemisuccinoyloxy-, 7.alpha.- and .beta.(I)-(.omega.-carboxy)-testosterones. The prepn. of an antigen is also described. Bovine serum albumin is conjugated to I using a std. method. Analysis (uv spectra) of the conjugate showed that the antigen contained 18% of the steroid acid (I).

## IT 59287-27-3P 59287-28-4P

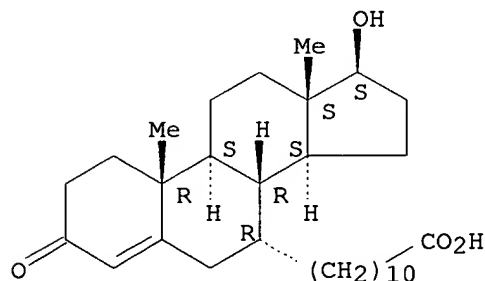
RL: PREP (Preparation)

(haptens, prepn. and use of, in antigens prepn.)

RN 59287-27-3 HCAPLUS

CN Androst-4-ene-7-undecanoic acid, 17-hydroxy-3-oxo-, (7.alpha.,17.beta.)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 59287-28-4 HCAPLUS

CN Androst-4-ene-7-undecanoic acid, 17-hydroxy-3-oxo-, (7.beta.,17.beta.)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

